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PASSWORD:
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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 20	EVENTLINE will be removed from STN
NEWS 28	Mar 24	PATDPAFULL now available on STN
NEWS 29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 30	Apr 11	Display formats in DGENE enhanced
NEWS 31	Apr 14	MEDLINE Reload
NEWS 32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 33	Jun 13	Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS 34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35	Apr 28	RDISCLOSURE now available on STN
NEWS 36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 38	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39	May 16	CHEMREACT will be removed from STN
NEWS 40	May 19	Simultaneous left and right truncation added to WSCA

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 NEWS 41  May 19  RAPRA enhanced with new search field, simultaneous left and
                  right truncation
 NEWS 42  Jun 06  Simultaneous left and right truncation added to CBNB
 NEWS 43  Jun 06  PASCAL enhanced with additional data
 NEWS 44  Jun 20  2003 edition of the FSTA Thesaurus is now available

 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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FILE 'HOME' ENTERED AT 13:28:41 ON 21 JUN 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 13:28:51 ON 21 JUN 2003
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES:   20 JUN 2003  HIGHEST RN 534773-28-9
DICTIONARY FILE UPDATES:  20 JUN 2003  HIGHEST RN 534773-28-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10018688.1
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L1 STRUCTURE UPLOADED

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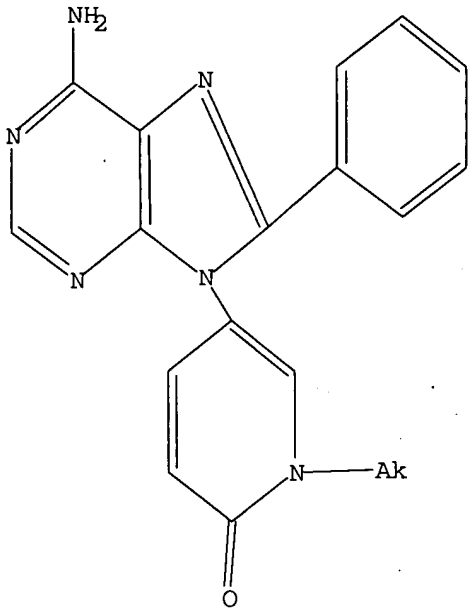
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:29:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 13:29:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 50 TO ITERATE

100.0% PROCESSED 50 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

L3 25 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	148.15	148.36

FILE 'CAPLUS' ENTERED AT 13:29:24 ON 21 JUN 2003
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FILE COVERS 1907 - 21 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 20 Jun 2003 (20030620/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d l4 fbib hitstr abs total

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
AN 2001:31502 CAPLUS
DN 134:100881
TI Preparation of fused imidazole compounds and remedies for diabetes mellitus
IN Asano, Osamu; Harada, Hitoshi; Yoshikawa, Seiji; Watanabe, Nobuhisa; Inoue, Takashi; Horizoe, Tatsuo; Yasuda, Nobuyuki; Oohashi, Kaya; Minami, Hiroe; Nagaoka, Junsaku; Murakami, Manabu; Kobayashi, Seiichi; Tanaka, Isao; Kawata, Tsutomu; Shimomura, Naoyuki; Akamatsu, Hirofumi; Ozeki, Naoki; Shimizu, Toshikazu; Hayashi, Kenji; Haga, Toyokazu; Negi, Shigeto; Naito, Toshihiko
PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002400	A1	20010111	WO 2000-JP4358	20000630
	W: AU, BR, CA, CN, HU, IL, JP, KR, MX, NO, NZ, RU, US, ZA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
				JP 1999-188484 A	19990702
				JP 2000-143495 A	20000516
				JP 2000-182786 A	20000619
	AU 2000055717	A5	20010122	AU 2000-55717	20000630

JP 1999-188484 A 19990702
JP 2000-143495 A 20000516
JP 2000-182786 A 20000619
WO 2000-JP4358 W 20000630

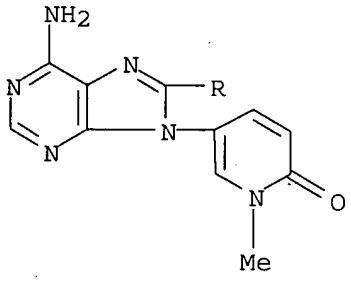
EP 1221444 A1 20020710 EP 2000-940909 20000630
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY

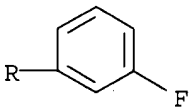
JP 1999-188484 A 19990702
JP 2000-143495 A 20000516
JP 2000-182786 A 20000619
WO 2000-JP4358 W 20000630

OS MARPAT 134:100881

IT **318468-14-3P 318468-15-4P 318468-21-2P**
318468-44-9P 318468-45-0P 318468-46-1P
318468-48-3P 318468-49-4P 318468-50-7P
318468-51-8P 318468-52-9P 318468-53-0P
318468-56-3P 318468-57-4P 318468-58-5P
318468-59-6P 318468-60-9P 318468-61-0P
318468-62-1P 318468-63-2P 318468-64-3P
318468-65-4P 318468-72-3P 318468-96-1P
318468-97-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of fused imidazole compds. as antagonists of adenosine A2 receptors and remedies for diabetes mellitus)

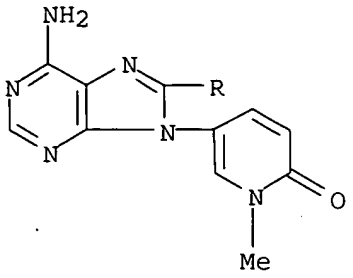
RN 318468-14-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

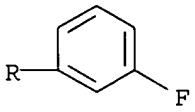




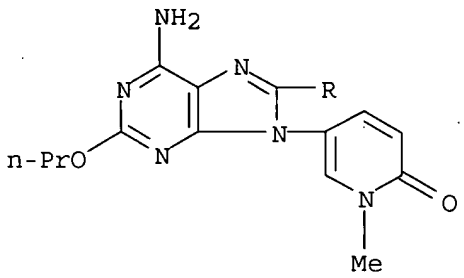
● HCl

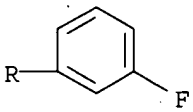
RN 318468-15-4 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)





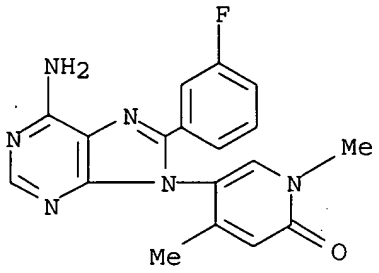
RN 318468-21-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-propoxy-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)





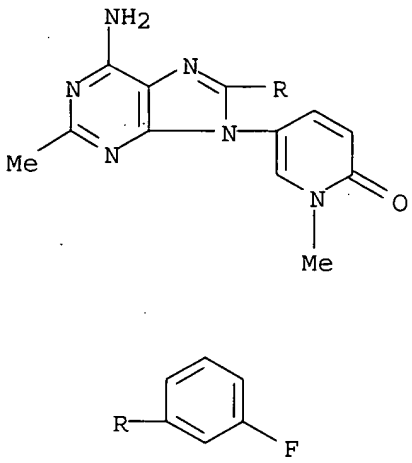
● HCl

RN 318468-44-9 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



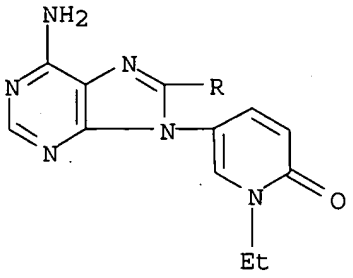
● HCl

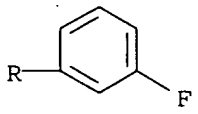
RN 318468-45-0 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-methyl-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

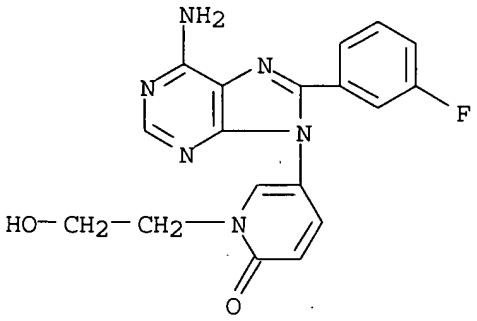
RN 318468-46-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



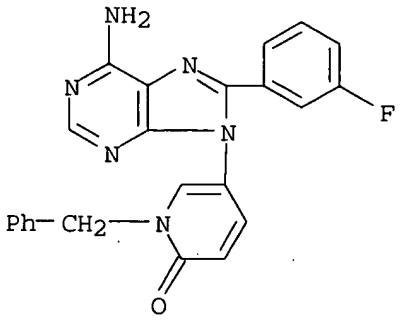


● HCl

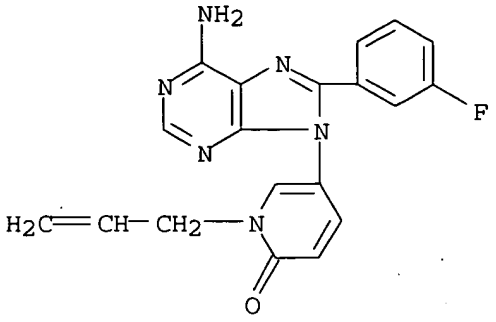
RN 318468-48-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



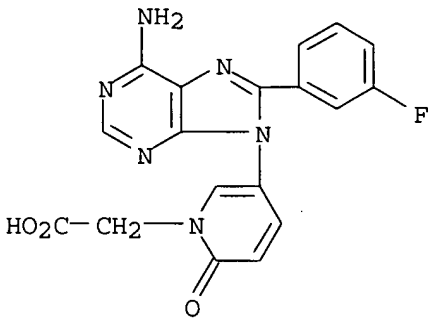
RN 318468-49-4 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



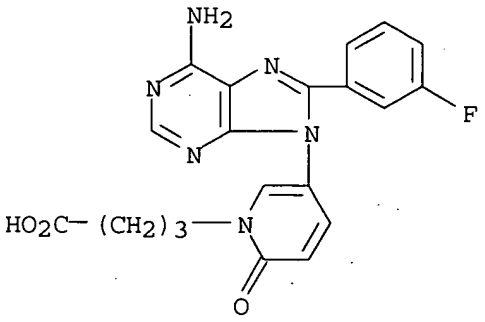
RN 318468-50-7 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-(2-propenyl)- (9CI) (CA INDEX NAME)



RN 318468-51-8 CAPLUS
CN 1(2H)-Pyridineacetic acid, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-2-oxo- (9CI) (CA INDEX NAME)



RN 318468-52-9 CAPLUS
CN 1(2H)-Pyridinebutanoic acid, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-2-oxo- (9CI) (CA INDEX NAME)



RN 318468-53-0 CAPLUS
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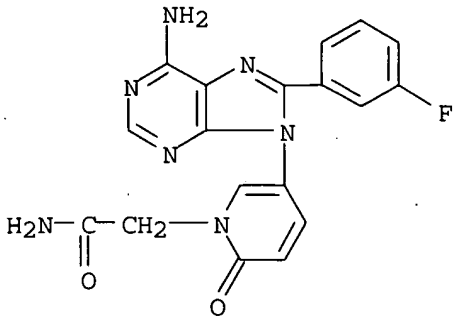
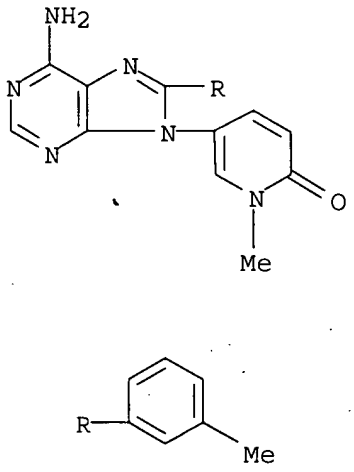
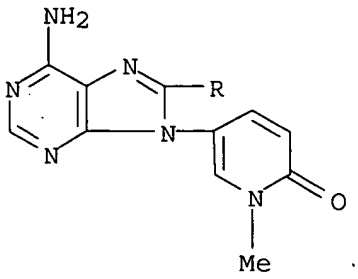


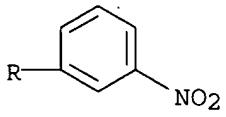
RN 318468-56-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-methylphenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

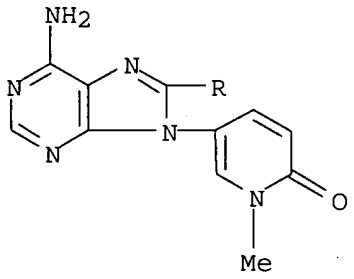
RN 318468-57-4 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-nitrophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

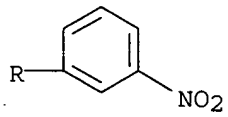




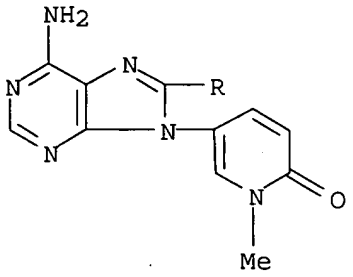
● HCl

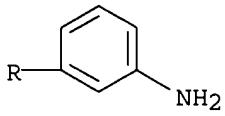
RN 318468-58-5 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-nitrophenyl)-9H-purin-9-yl]-1-methyl-
(9CI) (CA INDEX NAME)





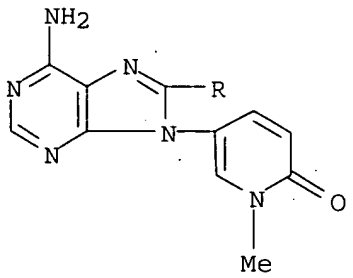
RN 318468-59-6 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-aminophenyl)-9H-purin-9-yl]-1-methyl-,
dihydrochloride (9CI) (CA INDEX NAME)

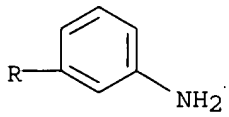




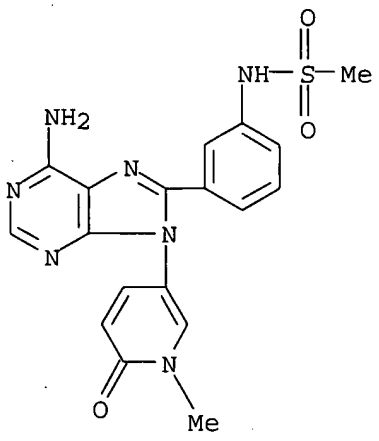
● 2 HCl

RN 318468-60-9 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-aminophenyl)-9H-purin-9-yl]-1-methyl-(9CI) (CA INDEX NAME)



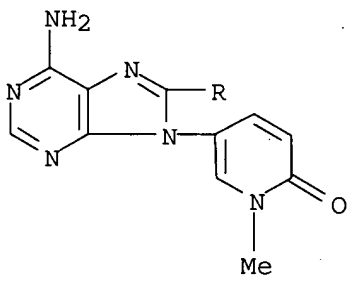


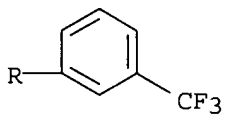
RN 318468-61-0 CAPLUS
CN Methanesulfonamide, N-[3-[6-amino-9-(1,6-dihydro-1-methyl-6-oxo-3-pyridinyl)-9H-purin-8-yl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

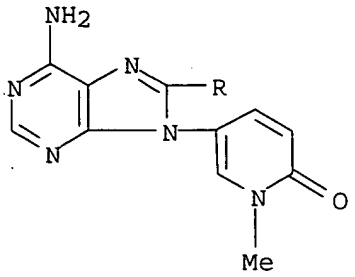
RN 318468-62-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-[3-(trifluoromethyl)phenyl]-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

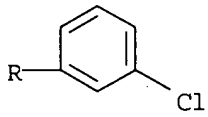




● HCl

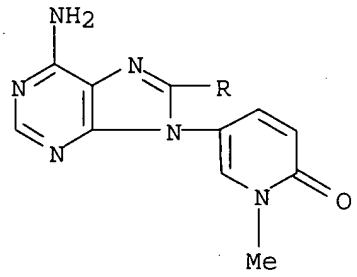
RN 318468-63-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-chlorophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

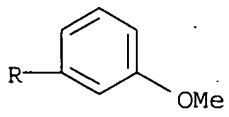




● HCl

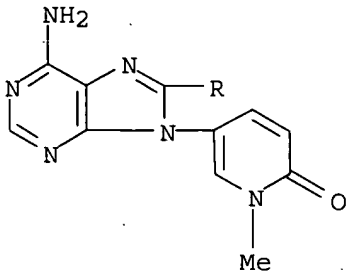
RN 318468-64-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-methoxyphenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

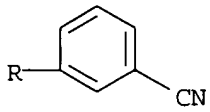




● HCl

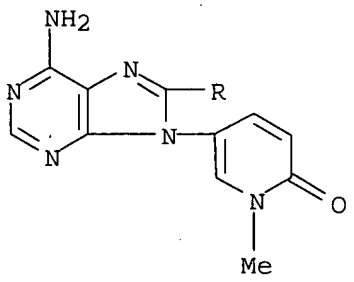
RN 318468-65-4 CAPLUS
CN Benzonitrile, 3-[6-amino-9-(1,6-dihydro-1-methyl-6-oxo-3-pyridinyl)-9H-purin-8-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

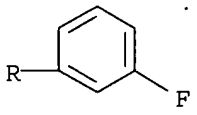




● HCl

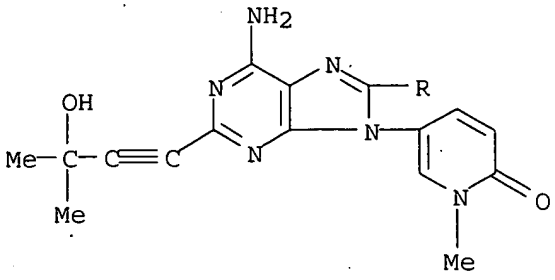
RN 318468-72-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-, dihydrate (9CI) (CA INDEX NAME)

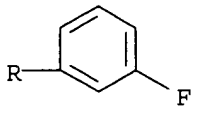




●2 H_2O

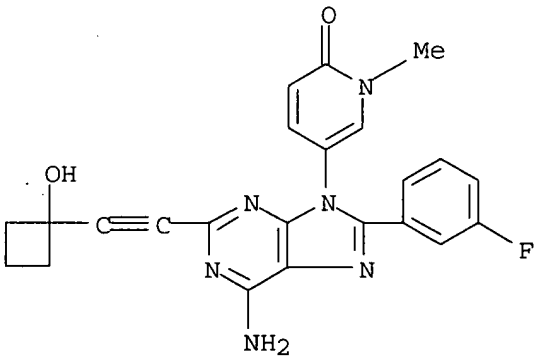
RN 318468-96-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-(3-hydroxy-3-methyl-1-butynyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)





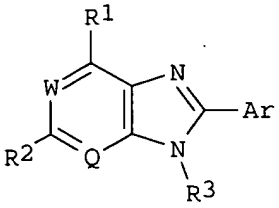
● HCl

RN 318468-97-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclobutyl)ethynyl]-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

GI



I

AB Novel fused imidazole compds. such as purine derivs. of general formula (I), pharmacol. acceptable salts thereof, or hydrates of both [wherein R1 = H, OH, halo, (un)substituted C1-8 alkyl, (un)substituted NH2; R2 = H, halo, (un)substituted NH2, (un)substituted C2-8 alkenyl, (un)substituted C3-8 alkynyl, (un)substituted C1-8 alkyl; R3 = (un)substituted C3-8 alkynyl, C3-8 alkenyl, (un)substituted C1-8 alkyl, (un)substituted aryl, (un)substituted heteroaryl, etc.; Ar = (un)substituted aryl, (un)substituted heteroaryl, optionally halo- or C1-6 alkyl-substituted N-C1-6 alkyl- or N-C3-6 cycloalkyl-oxopyridyl or -oxopyrimidyl; Q, W = N, CH; some proviso are given] are prepd. These compds. exhibit adenosine A2 receptor antagonism and are effective in the prevention and treatment of diabetes mellitus and complications of diabetes. Thus, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1,2-dihydro-2-pyridinone was condensed with N,N-dimethylformamide di-Me acetal in DMF at room temp. for 1 h, ice-cooled, treated with NaH at 0-6.degree. for 30 min, and methylated by Me iodide at room temp. for 16 h to give 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-1,2-dihydro-2-pyridinone (II). II.HCl at 10 mg/kg p.o. in spontaneously diabetic mice lowered the blood sugar level to 47.3.+-.7.2% of the control animal.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d cost

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
CONNECT CHARGES	0.68	1.17
NETWORK CHARGES	0.12	0.24
SEARCH CHARGES	0.00	147.75
DISPLAY CHARGES	4.32	4.32
	5.12	153.48
CAPLUS FEE (5%)	0.25	0.25
FULL ESTIMATED COST	5.37	153.73

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.65	-0.65

IN FILE 'CAPLUS' AT 13:30:49 ON 21 JUN 2003

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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 NEWS 41  May 19  RAPRA enhanced with new search field, simultaneous left and
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 NEWS 44  Jun 20  2003 edition of the FSTA Thesaurus is now available

 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:37:37 ON 21 JUN 2003

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.21       0.21

FILE 'REGISTRY' ENTERED AT 13:37:47 ON 21 JUN 2003
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STRUCTURE FILE UPDATES:   20 JUN 2003  HIGHEST RN 534773-28-9
DICTIONARY FILE UPDATES:  20 JUN 2003  HIGHEST RN 534773-28-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10018688.3
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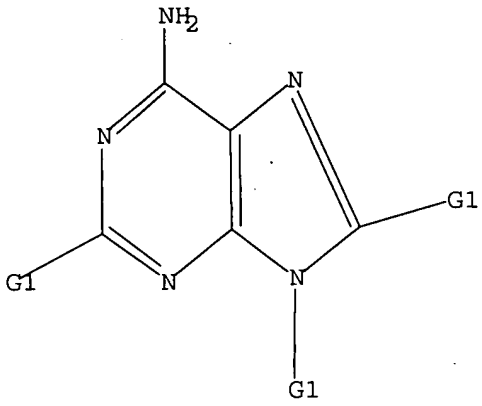
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:38:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4902 TO ITERATE

20.4% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 93844 TO 102236
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 13:38:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 100017 TO ITERATE

100.0% PROCESSED 100017 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.05

L3 0 SEA SSS FUL L1

=> log y
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 148.15 148.36

STN INTERNATIONAL LOGOFF AT 13:38:36 ON 21 JUN 2003

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:43:39 ON 21 JUN 2003

=> file reg
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                             0.21       0.21

FILE 'REGISTRY' ENTERED AT 13:43:49 ON 21 JUN 2003
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STRUCTURE FILE UPDATES:   20 JUN 2003  HIGHEST RN 534773-28-9
DICTIONARY FILE UPDATES:  20 JUN 2003  HIGHEST RN 534773-28-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10018688.4
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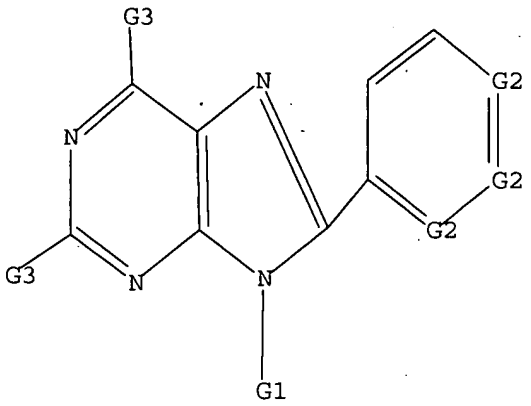
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 Cb,Cy,Hy

G2 N,CH

G3 C,O,N,OH,NH2,X,Cb,Cy,Ak,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:44:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 259 TO ITERATE

100.0% PROCESSED 259 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4215 TO 6145
PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 13:44:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5904 TO ITERATE

100.0% PROCESSED 5904 ITERATIONS 137 ANSWERS
SEARCH TIME: 00.00.01

L3 137 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.15	148.36

FILE 'CAPLUS' ENTERED AT 13:44:25 ON 21 JUN 2003

FILE COVERS 1907 - 21 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 20 Jun 2003 (20030620/ED)

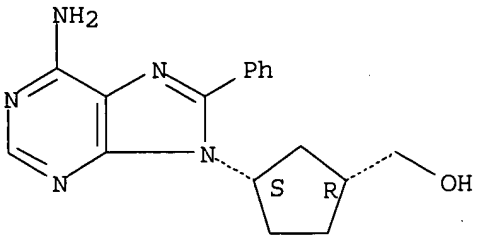
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 19 L3

=> d l4 fbib hitstr abs total

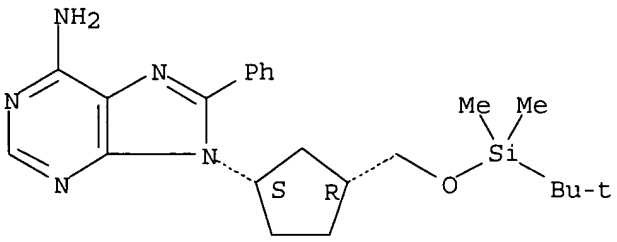
L4 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 2003:3721 CAPLUS
DN 138:338396
TI Synthesis of novel 8-substituted carbocyclic analogs of 2',3'-dideoxyadenosine with activity against hepatitis B virus
AU Gudmundsson, Kristjan S.; Daluge, Susan M.; Condreay, Lynn D.; Johnson, Lance C.
CS Division of Chemistry, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA
SO Nucleosides, Nucleotides & Nucleic Acids (2002), 21(11 & 12), 891-901
CODEN: NNNAFY; ISSN: 1525-7770
PB Marcel Dekker, Inc.
DT Journal
LA English
IT **515826-78-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of novel carbocyclic analogs of dideoxyadenosine with activity against hepatitis B virus)
RN 515826-78-5 CAPLUS
CN Cyclopentanemethanol, 3-(6-amino-8-phenyl-9H-purin-9-yl)-, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **515826-72-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of novel carbocyclic analogs of dideoxyadenosine with activity against hepatitis B virus)
RN 515826-72-9 CAPLUS
CN 9H-Purin-6-amine, 9-[(1S,3R)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]cyclopentyl]-8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

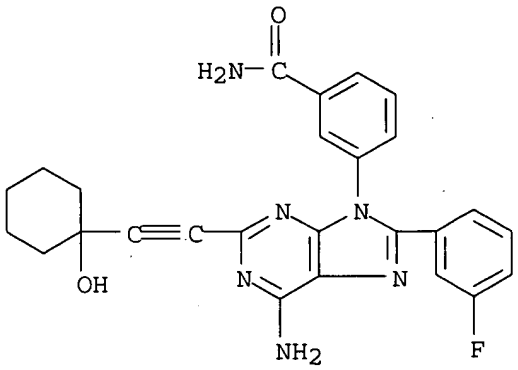


AB Synthesis and antiviral activity of several new 8-substituted carbocyclic analogs of D-2',3'-dideoxyadenosine are described. The new 8-substituted analogs were synthesized via lithiation of carbocyclic 2',3'-dideoxyadenosine followed by quenching with electrophiles. This methodol. allows for a divergent synthesis of a variety of 8-substituted analogs from carbocyclic 2',3'-dideoxyadenosine in high yields. 8-Me and 8-halogenated carbocyclic 2',3'-dideoxyadenosine analogs showed 6-25 fold more activity against hepatitis B virus than the unsubstituted carbocyclic D-2',3'-dideoxyadenosine.
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 2001:667342 CAPLUS
DN 136:112192
TI 2-Alkynyl-8-aryladenines possessing an amide moiety: their synthesis and structure-activity relationships of effects on hepatic glucose production induced via agonism of the A2B adenosine receptor
AU Harada, H.; Asano, O.; Kawata, T.; Inoue, T.; Horizoe, T.; Yasuda, N.; Nagata, K.; Murakami, M.; Nagaoka, J.; Kobayashi, S.; Tanaka, I.; Abe, S.
CS Tsukuba Research Laboratories, Eisai Company, Ltd., Tsukuba, Ibaraki, 300-2635, Japan
SO Bioorganic & Medicinal Chemistry (2001), 9(10), 2709-2726
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English

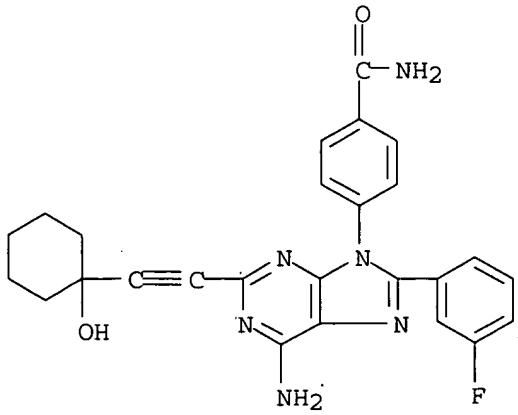
IT **232252-56-1P 232252-57-2P 391248-58-1P**
391248-59-2P 391248-60-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure activity of alkynylaryladenines as A2A adenosine receptor agonists and effects on hepatic glucose prodn.)

RN 232252-56-1 CAPLUS
CN Benzamide, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

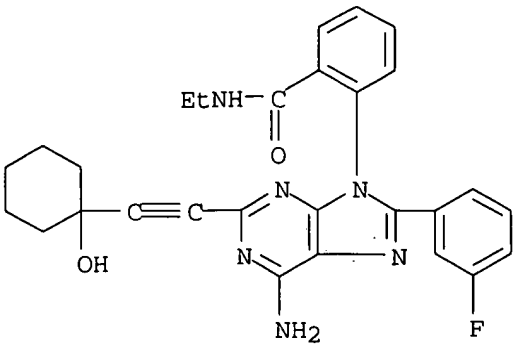
RN 232252-57-2 CAPLUS
CN Benzamide, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

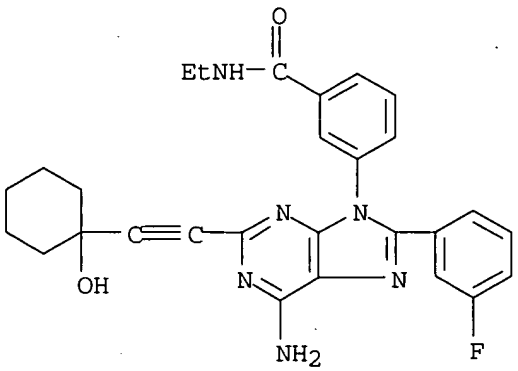
RN 391248-58-1 CAPLUS
CN Benzamide, 2-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-

9H-purin-9-yl]-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



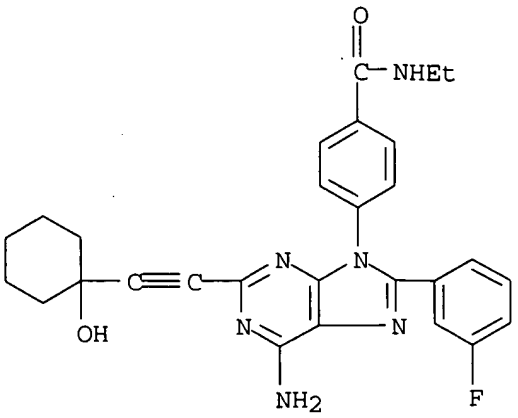
● HCl

RN 391248-59-2 CAPLUS
CN Benzamide, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

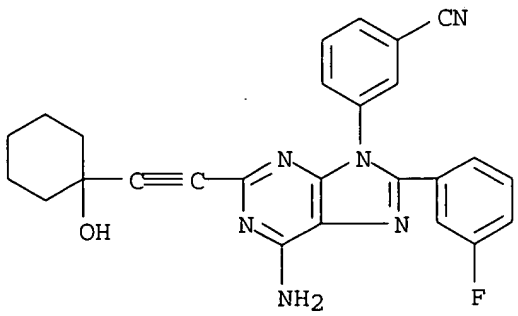
RN 391248-60-5 CAPLUS
CN Benzamide, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



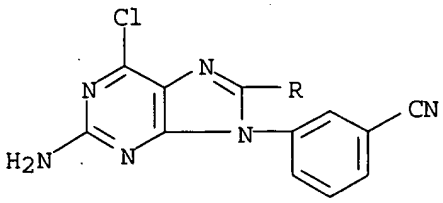
● HCl

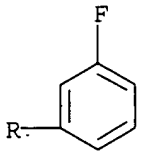
IT **232252-44-7P 232254-90-9P 232254-91-0P**
232254-92-1P 391249-14-2P 391249-15-3P
391249-16-4P 391249-17-5P 391249-21-1P
391249-22-2P 391249-23-3P 391249-24-4P
391249-25-5P 391249-29-9P 391249-30-2P
391249-31-3P 391249-32-4P 391249-33-5P
391249-37-9P 391249-38-0P 391249-39-1P
391249-40-4P 391249-41-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and structure activity of alkynylaryladenines as A2A adenosine receptor agonists and effects on hepatic glucose prodn.)

RN 232252-44-7 CAPLUS
CN Benzonitrile, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)

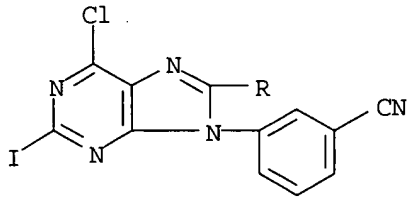


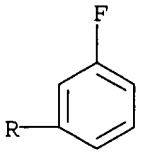
RN 232254-90-9 CAPLUS
CN Benzonitrile, 3-[2-amino-6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



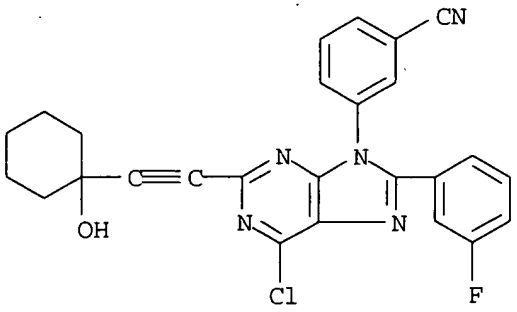


RN 232254-91-0 CAPLUS
CN Benzonitrile, 3-[6-chloro-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



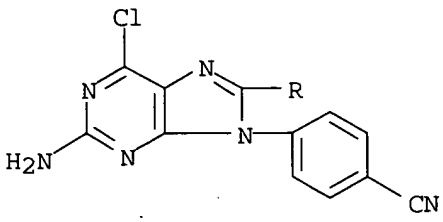


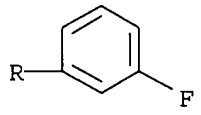
RN 232254-92-1 CAPLUS
CN Benzonitrile, 3-[6-chloro-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



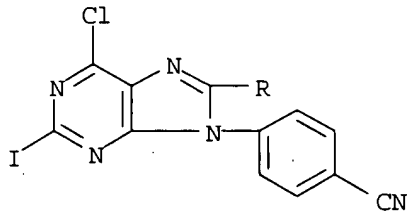
RN 391249-14-2 CAPLUS

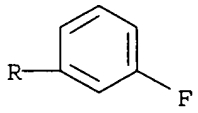
CN Benzonitrile, 4-[2-amino-6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



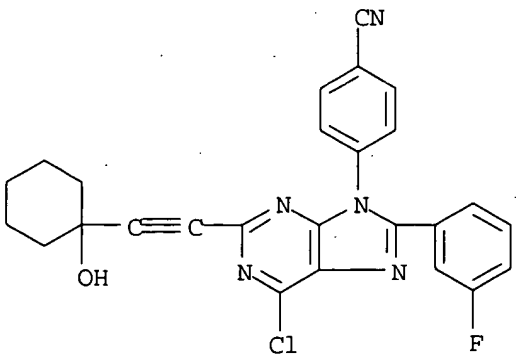


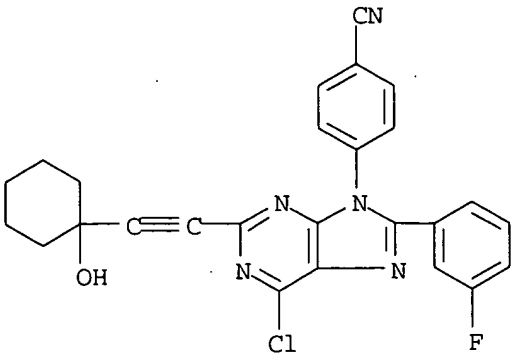
RN 391249-15-3 CAPLUS
CN Benzonitrile, 4-[6-chloro-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



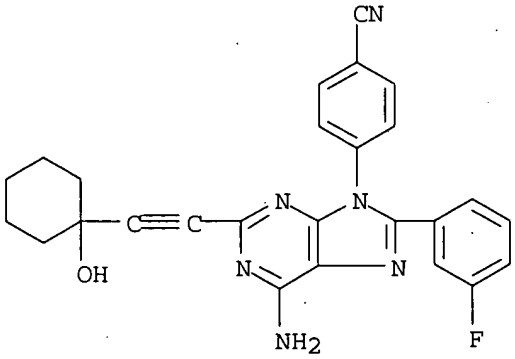


RN 391249-16-4 CAPLUS
CN Benzonitrile, 4-[6-chloro-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)

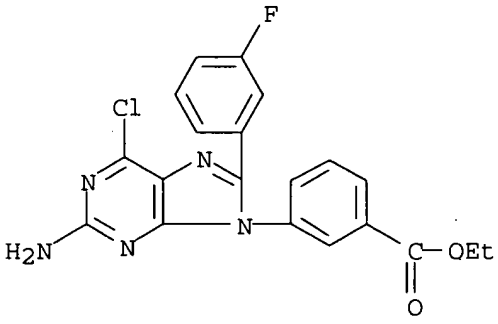




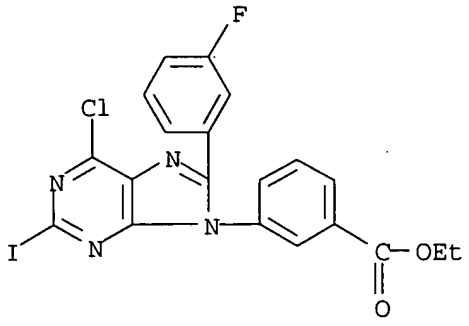
RN 391249-17-5 CAPLUS
CN Benzonitrile, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



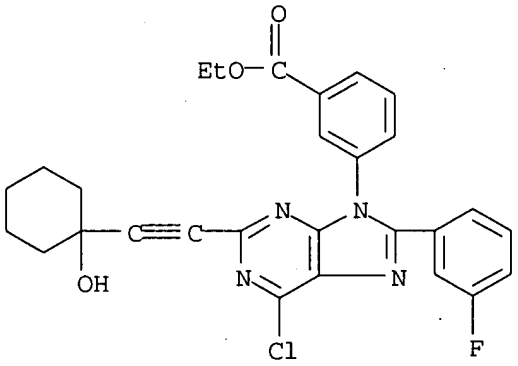
RN 391249-21-1 CAPLUS
CN Benzoic acid, 3-[2-amino-6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



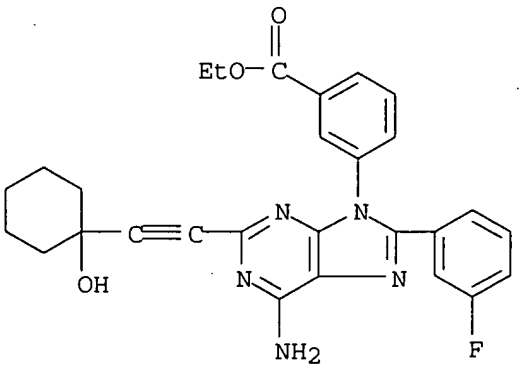
RN 391249-22-2 CAPLUS
CN Benzoic acid, 3-[6-chloro-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



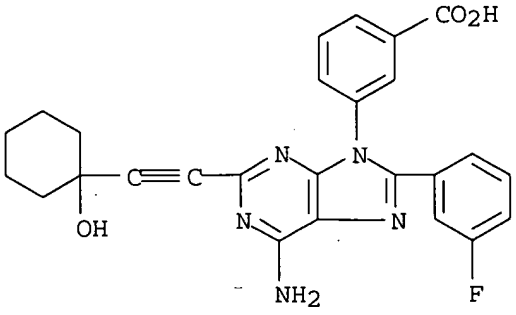
RN 391249-23-3 CAPLUS
CN Benzoic acid, 3-[6-chloro-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



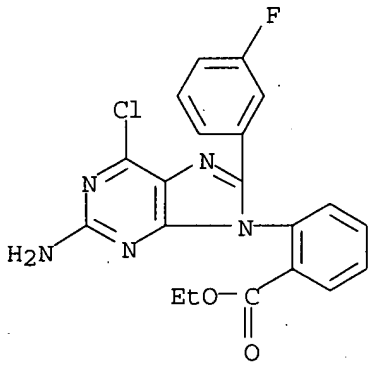
RN 391249-24-4 CAPLUS
CN Benzoic acid, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



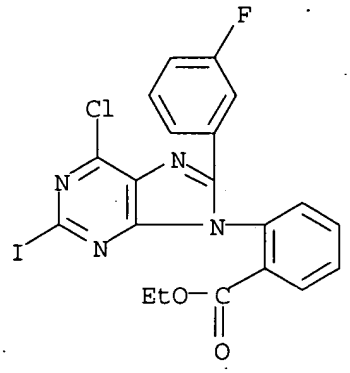
RN 391249-25-5 CAPLUS
CN Benzoic acid, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



RN 391249-29-9 CAPLUS
CN Benzoic acid, 2-[2-amino-6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)

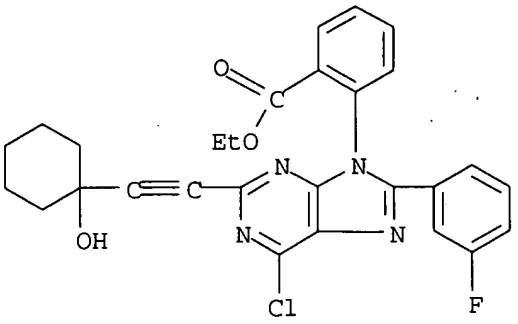


RN 391249-30-2 CAPLUS
CN Benzoic acid, 2-[6-chloro-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)

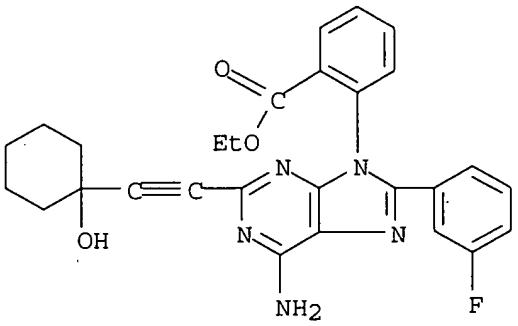


RN 391249-31-3 CAPLUS
CN Benzoic acid, 2-[6-chloro-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX

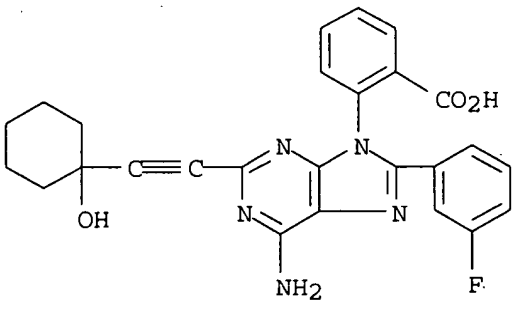
NAME)



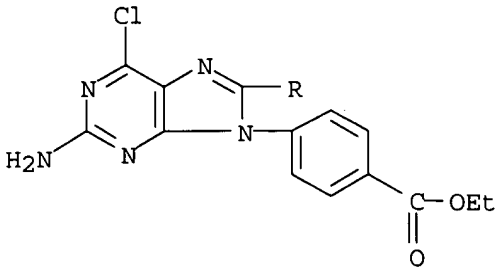
RN 391249-32-4 CAPLUS
CN Benzoic acid, 2-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)

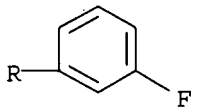


RN 391249-33-5 CAPLUS
CN Benzoic acid, 2-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)

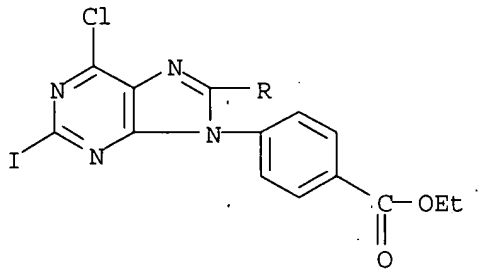


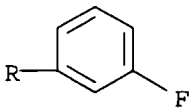
RN 391249-37-9 CAPLUS
CN Benzoic acid, 4-[2-amino-6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



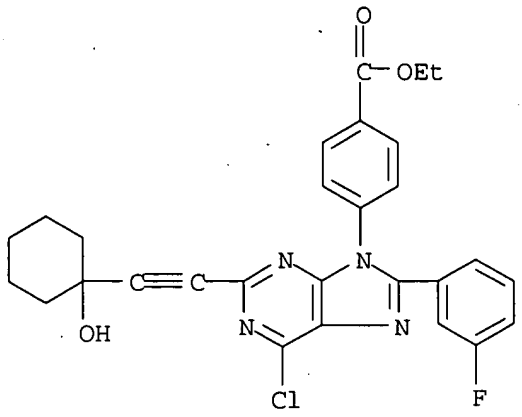


RN 391249-38-0 CAPLUS
CN Benzoic acid, 4-[6-chloro-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)

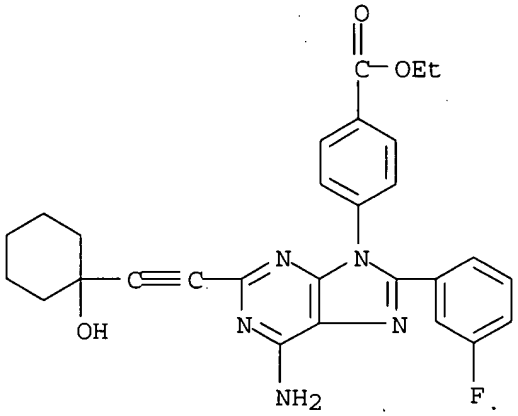




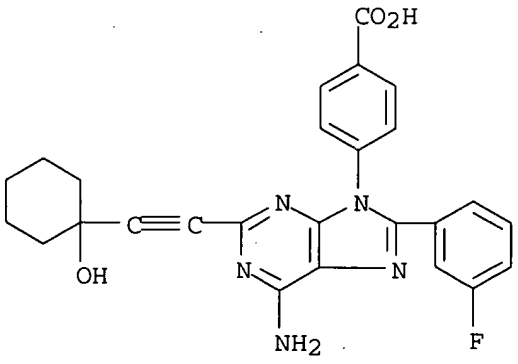
RN 391249-39-1 CAPLUS
CN Benzoic acid, 4-[6-chloro-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



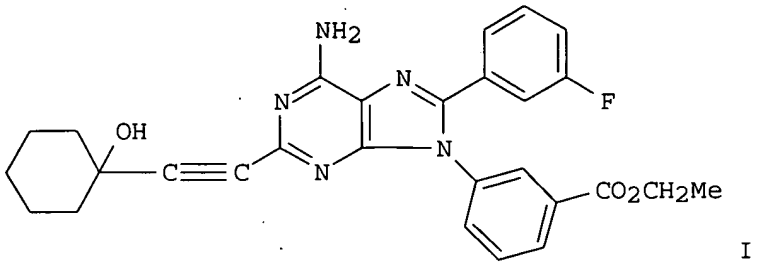
RN 391249-40-4 CAPLUS
CN Benzoic acid, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 391249-41-5 CAPLUS
CN Benzoic acid, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



GI

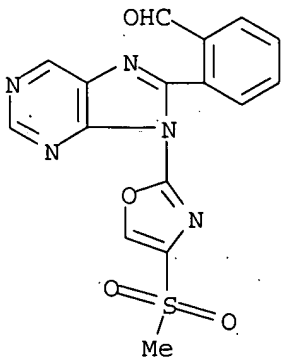


I

AB A series of 2-alkynyl-8-aryladenine derivs. bearing an amide moiety at the 9-position of adenine was synthesized. These analogs were evaluated for inhibitory activity on N-ethylcarboxamidoadenosine (NECA)-induced glucose prodn. in primary cultured rat hepatocytes. The m-primary benzamide deriv. (I) was the most potent compd. (IC50=0.017 .mu.M), being 15-fold more active than the corresponding 9-Me deriv. I showed 72- and 5.2-fold selectivity for human A2B receptor vs. human A1 and A2A receptors, resp. Structure-activity relation (SAR) studies of the synthesized compds. indicated that a three-carbon linker, fixed in the form of a benzene ring, between the adenine core and the amide moiety is important for both A2B antagonistic activity and selectivity. The IC50 values in rat hepatocyte glucose assay correlated well with the IC50 values in cAMP assay using Chinese hamster ovary cells stably transfected with human A2B receptors (r2 = 0.94). The A1 and A2A affinities showed no correlation with the potency to inhibit NECA-induced glucose prodn. These results strongly support the previous conclusion that adenosine agonist-induced hepatic glucose prodn. in rat hepatocytes is mediated through the A2B receptor.

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 2001:400641 CAPLUS
DN 135:220646
TI Design of new selective inhibitors of cyclooxygenase-2 by dynamic assembly of molecular building blocks
AU Zhu, Jiang; Yu, Haibo; Fan, Hao; Liu, Haiyan; Shi, Yunyu
CS Laboratory of Structural Biology, School of Life Science, University of Science and Technology of China (USTC), Hefei, 230026, Peop. Rep. China
SO Journal of Computer-Aided Molecular Design (2001), 15(5), 447-463
CODEN: JCADEQ; ISSN: 0920-654X
PB Kluwer Academic Publishers
DT Journal
LA English
IT **359636-19-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design of new selective inhibitors of cyclooxygenase-2 by dynamic assembly of mol. building blocks)
RN 359636-19-4 CAPLUS
CN Benzaldehyde, 2-[9-[4-(methylsulfonyl)-2-oxazolyl]-9H-purin-8-yl]- (9CI) (CA INDEX NAME)



AB A method of dynamically assembling mol. building blocks - DycoBlock - has been proposed and tested by Liu et al. [1]. This method is based on multiple-copy stochastic dynamics simulation in the presence of a receptor mol. In this method, a novel algorithm was used to dynamically assemble the mol. building blocks to form candidate compds. Currently, some new improvements have been incorporated into DycoBlock to make it more efficient. In the new version of DycoBlock, the binding energy and solvent accessible surface area (SASA) can be used to screen the resulting compds. A simple clustering algorithm based on mol. similarity was developed and used to classify the remaining compds. The revised DycoBlock was tested by breaking SC-558 - a selective inhibitor of cyclooxygenase-2 (COX-2) - into building blocks and reassembling them in the active site of the enzyme. The accuracy of recovery grew to 58.8% while it was only 16.7% in the previous version. Then, thirty-three kinds of mol. building blocks were used in the design of novel inhibitors and the investigation of diversity. As a result, a total of 1441 compds. was generated with high diversity. After the first screening procedure, there remained 864 reasonable compds. The results from clustering indicate that the structural motifs in the diarylheterocycle class of COX-2-selective inhibitors [2] have been generated using the revised DycoBlock, and their binding modes were investigated.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 2001:31502 CAPLUS
DN 134:100881
TI Preparation of fused imidazole compounds and remedies for diabetes mellitus
IN Asano, Osamu; Harada, Hitoshi; Yoshikawa, Seiji; Watanabe, Nobuhisa; Inoue, Takashi; Horizoe, Tatsuo; Yasuda, Nobuyuki; Oohashi, Kaya; Minami, Hiroe; Nagaoka, Junsaku; Murakami, Manabu; Kobayashi, Seiichi; Tanaka, Isao; Kawata, Tsutomu; Shimomura, Naoyuki; Akamatsu, Hirofumi; Ozeki, Naoki; Shimizu, Toshikazu; Hayashi, Kenji; Haga, Toyokazu; Negi, Shigeto; Naito, Toshihiko
PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002400	A1	20010111	WO 2000-JP4358	20000630
	W: AU, BR, CA, CN, HU, IL, JP, KR, MX, NO, NZ, RU, US, ZA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
				JP 1999-188484 A	19990702
				JP 2000-143495 A	20000516
				JP 2000-182786 A	20000619
	AU 2000055717	A5	20010122	AU 2000-55717	20000630
				JP 1999-188484 A	19990702
				JP 2000-143495 A	20000516
				JP 2000-182786 A	20000619
				WO 2000-JP4358 W	20000630
	EP 1221444	A1	20020710	EP 2000-940909	20000630
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
				JP 1999-188484 A	19990702
				JP 2000-143495 A	20000516
				JP 2000-182786 A	20000619
				WO 2000-JP4358 W	20000630

OS MARPAT 134:100881

IT **318468-06-3P 318468-10-9P 318468-11-0P**
318468-12-1P 318468-13-2P 318468-14-3P
318468-15-4P 318468-16-5P 318468-17-6P
318468-21-2P 318468-22-3P 318468-23-4P
318468-24-5P 318468-35-8P 318468-44-9P
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318468-65-4P 318468-71-2P 318468-72-3P
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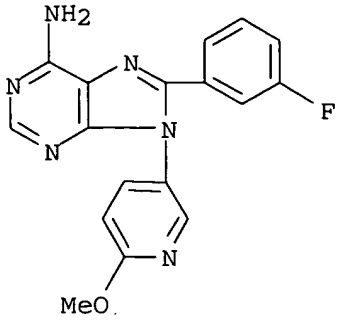
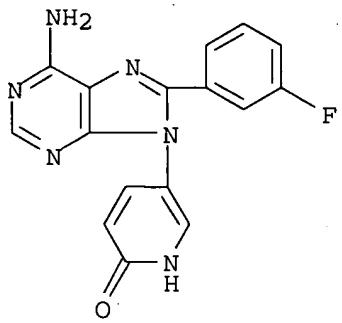
318468-88-1P 318468-95-0P 318468-96-1P
318468-97-2P 318468-98-3P 318469-02-2P
318469-03-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of fused imidazole compds. as antagonists of adenosine A2 receptors and remedies for diabetes mellitus)

RN 318468-06-3 CAPLUS

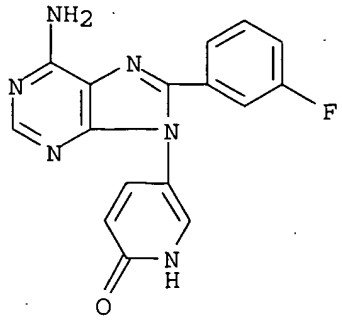
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-9-(6-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 318468-10-9 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]- (9CI) (CA INDEX NAME)

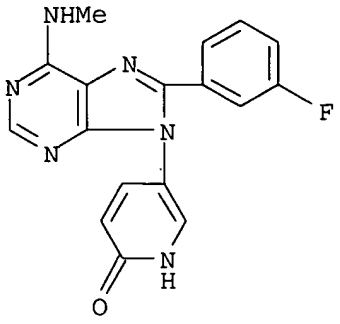


RN 318468-11-0 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



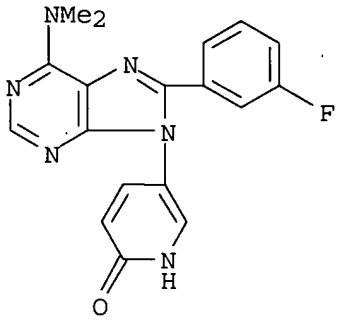
● HCl

RN 318468-12-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[8-(3-fluorophenyl)-6-(methylamino)-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



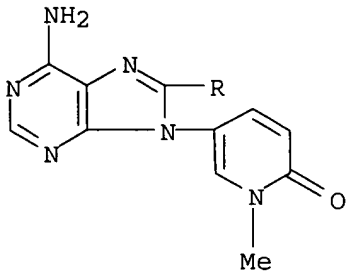
● HCl

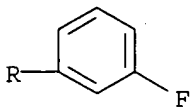
RN 318468-13-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-(dimethylamino)-8-(3-fluorophenyl)-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

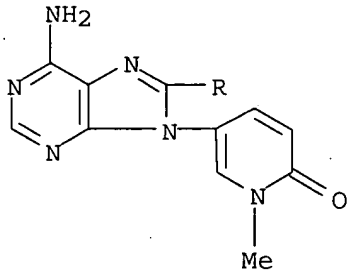
RN 318468-14-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

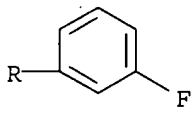




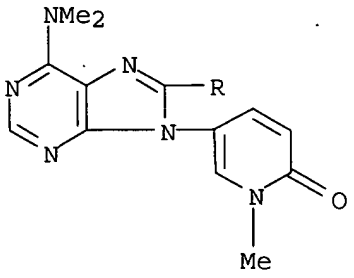
● HCl

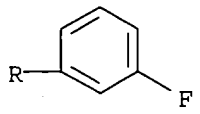
RN 318468-15-4 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-
(9CI) (CA INDEX NAME)





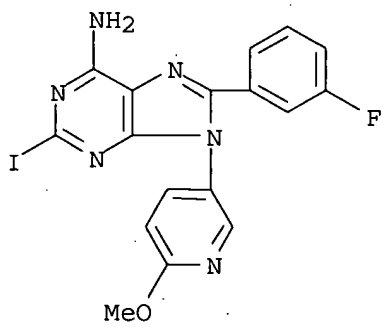
RN 318468-16-5 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-(dimethylamino)-8-(3-fluorophenyl)-9H-purin-9-yl]-1-
methyl-, monohydrochloride (9CI) (CA INDEX NAME)



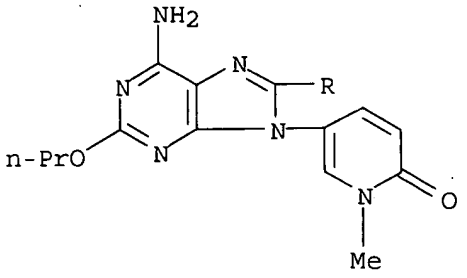


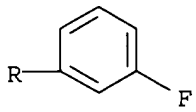
● HCl

RN 318468-17-6 CAPLUS
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-2-iodo-9-(6-methoxy-3-pyridinyl)-(9CI) (CA INDEX NAME)



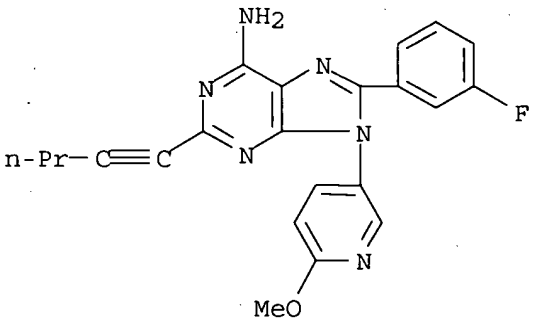
RN 318468-21-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-propoxy-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



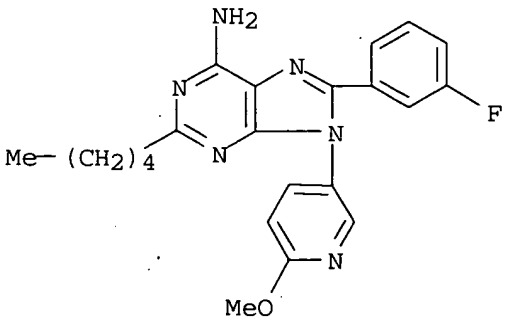


● HCl

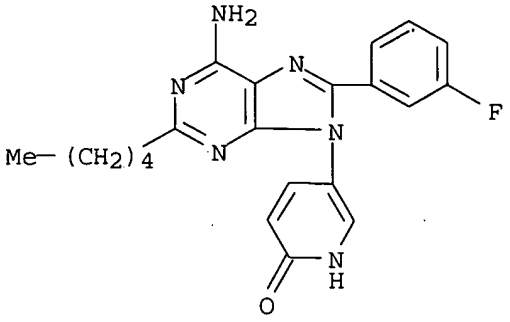
RN 318468-22-3 CAPLUS
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-9-(6-methoxy-3-pyridinyl)-2-(1-pentynyl)- (9CI) (CA INDEX NAME)



RN 318468-23-4 CAPLUS
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-9-(6-methoxy-3-pyridinyl)-2-pentyl- (9CI) (CA INDEX NAME)

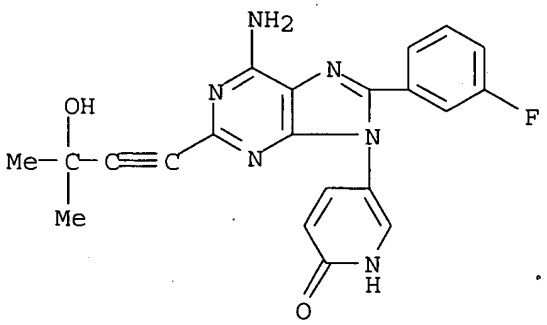


RN 318468-24-5 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-pentyl-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



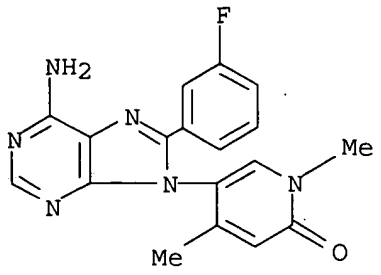
● HCl

RN 318468-35-8 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-(3-hydroxy-3-methyl-1-butynyl)-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



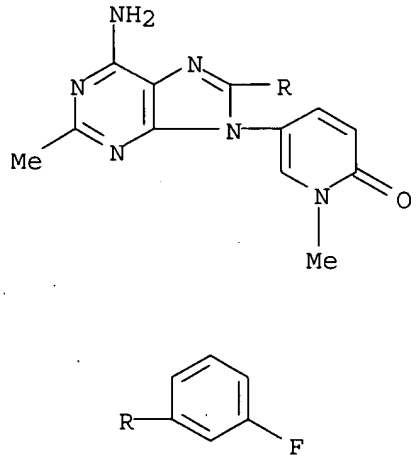
● HCl

RN 318468-44-9 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



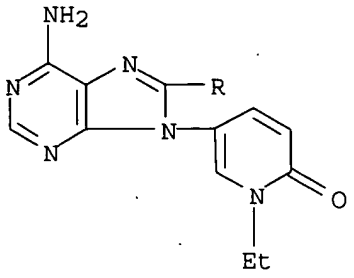
● HCl

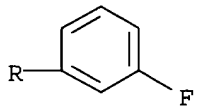
RN 318468-45-0 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-methyl-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

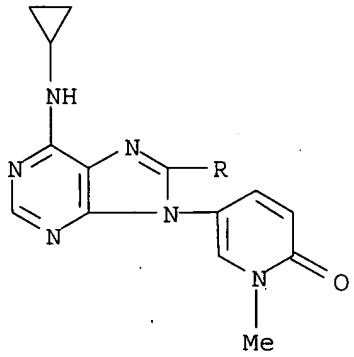
RN 318468-46-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)

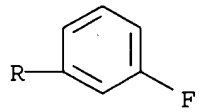




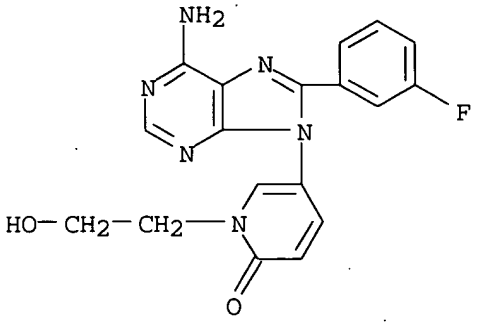
● HCl

RN 318468-47-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-(cyclopropylamino)-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)

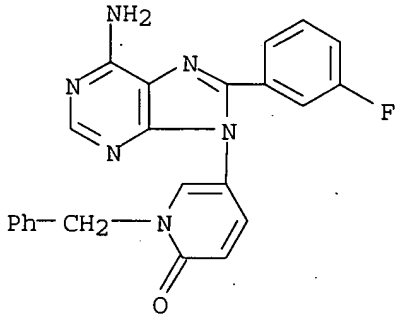




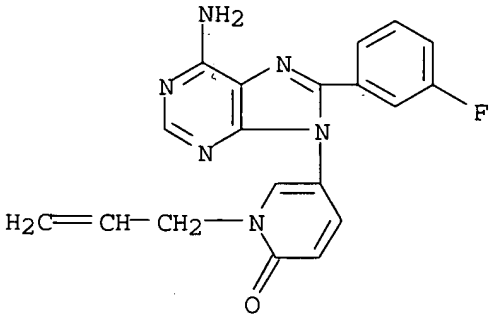
RN 318468-48-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



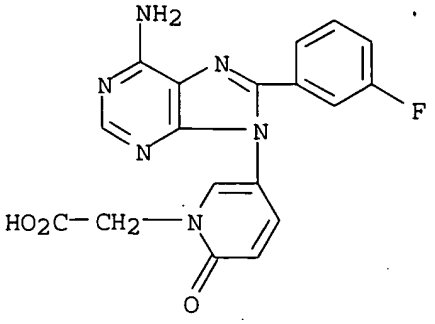
RN 318468-49-4 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



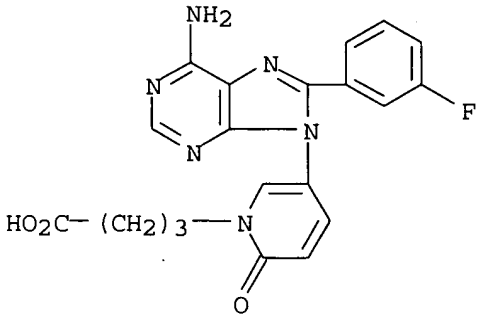
RN 318468-50-7 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-(2-propenyl)- (9CI) (CA INDEX NAME)



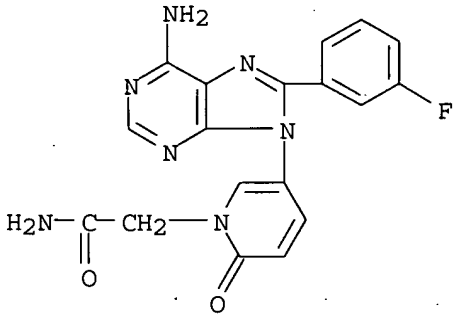
RN 318468-51-8 CAPLUS
CN 1(2H)-Pyridineacetic acid, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-2-oxo- (9CI) (CA INDEX NAME)



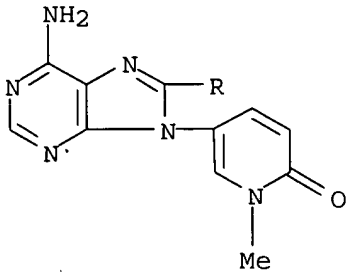
RN 318468-52-9 CAPLUS
CN 1(2H)-Pyridinebutanoic acid, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-2-oxo- (9CI) (CA INDEX NAME)

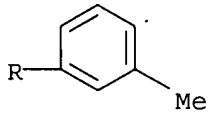


RN 318468-53-0 CAPLUS
CN 1(2H)-Pyridineacetamide, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-2-oxo- (9CI) (CA INDEX NAME)



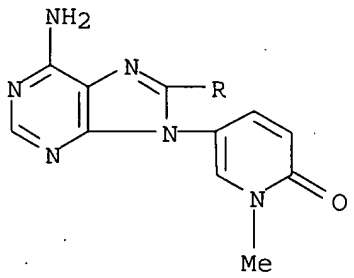
RN 318468-56-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-methylphenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

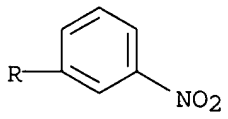




● HCl

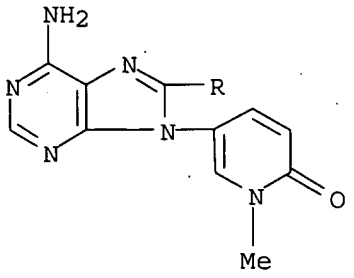
RN 318468-57-4 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-nitrophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

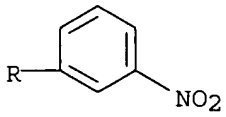




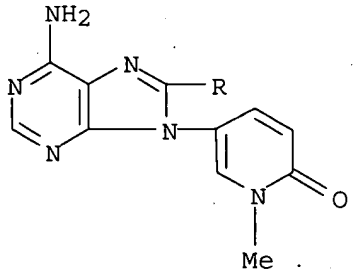
● HCl

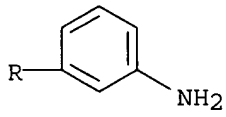
RN 318468-58-5 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-nitrophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)





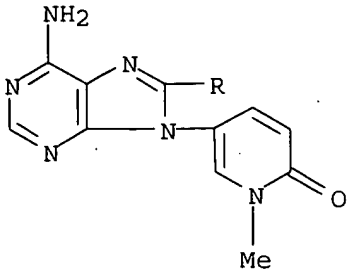
RN 318468-59-6 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-aminophenyl)-9H-purin-9-yl]-1-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

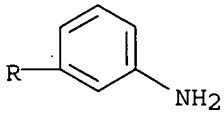




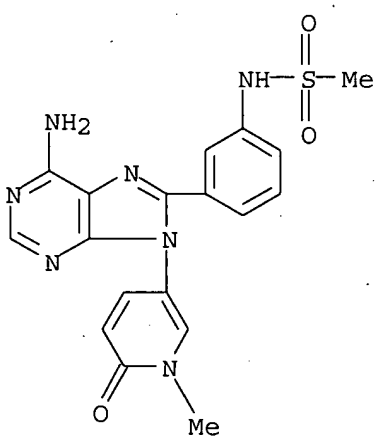
●2 HCl

RN 318468-60-9 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-aminophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)



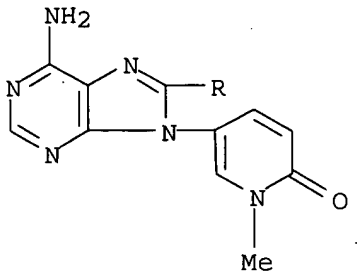


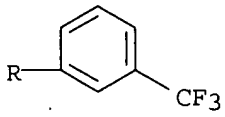
RN 318468-61-0 CAPLUS
CN Methanesulfonamide, N-[3-[6-amino-9-(1,6-dihydro-1-methyl-6-oxo-3-pyridinyl)-9H-purin-8-yl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

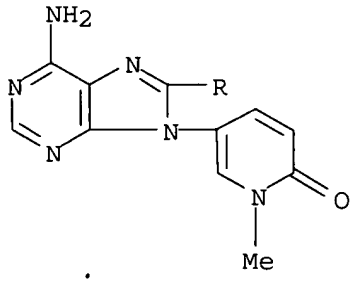
RN 318468-62-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-[3-(trifluoromethyl)phenyl]-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

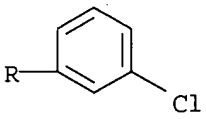




● HCl

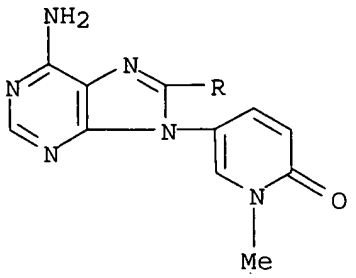
RN 318468-63-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-chlorophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

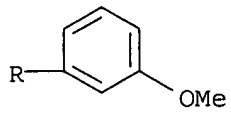




● HCl

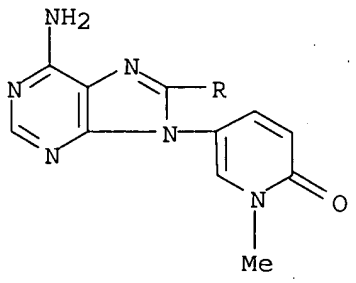
RN 318468-64-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-methoxyphenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

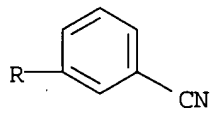




● HCl

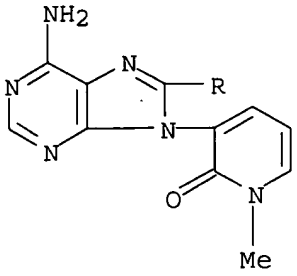
RN 318468-65-4 CAPLUS
CN Benzonitrile, 3-[6-amino-9-(1,6-dihydro-1-methyl-6-oxo-3-pyridinyl)-9H-purin-8-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

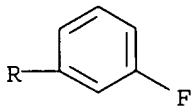




● HCl

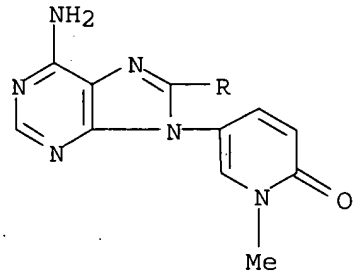
RN 318468-71-2 CAPLUS
CN 2(1H)-Pyridinone, 3-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

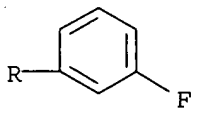




● HCl

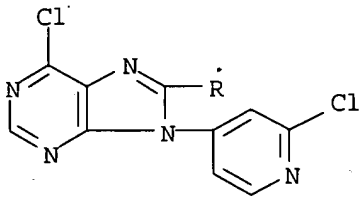
RN 318468-72-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-, dihydrate (9CI) (CA INDEX NAME)

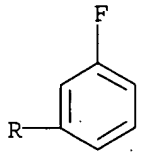




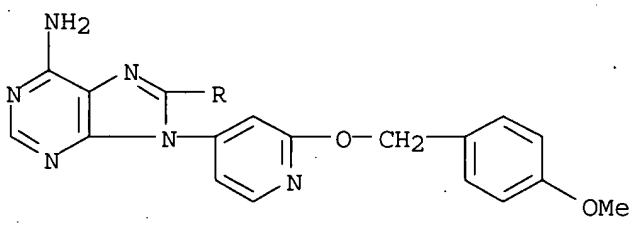
● 2 H_2O

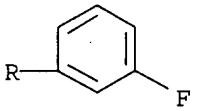
RN 318468-78-9 CAPLUS
CN 9H-Purine, 6-chloro-9-(2-chloro-4-pyridinyl)-8-(3-fluorophenyl)- (9CI) (CA INDEX NAME)



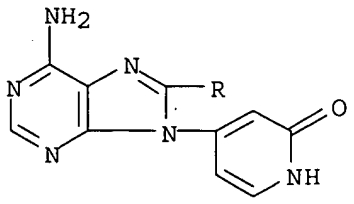


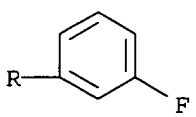
RN 318468-83-6 CAPLUS
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-9-[2-[(4-methoxyphenyl)methoxy]-4-pyridinyl]- (9CI) (CA INDEX NAME)



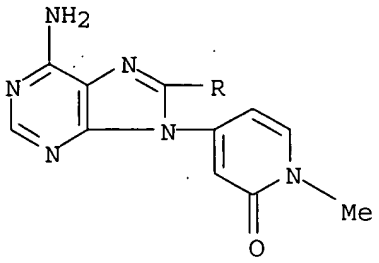


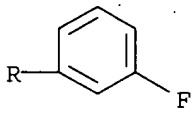
RN 318468-84-7 CAPLUS
CN 2(1H)-Pyridinone, 4-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



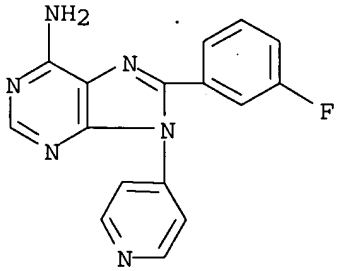


RN 318468-85-8 CAPLUS
CN 2(1H)-Pyridinone, 4-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)

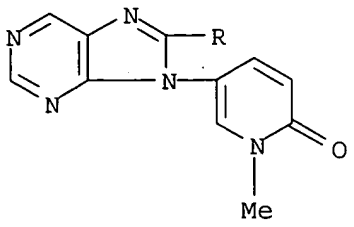


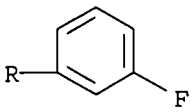


RN 318468-86-9 CAPLUS
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-9-(4-pyridinyl)- (9CI) (CA INDEX NAME)

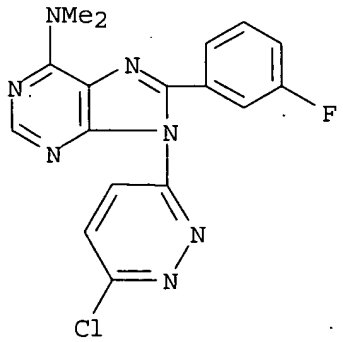


RN 318468-87-0 CAPLUS
CN 2(1H)-Pyridinone, 5-[8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)

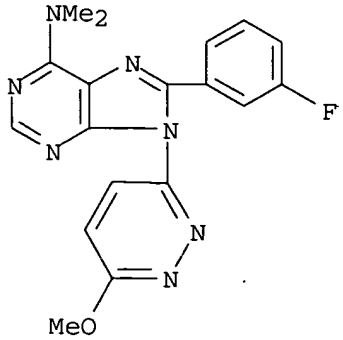




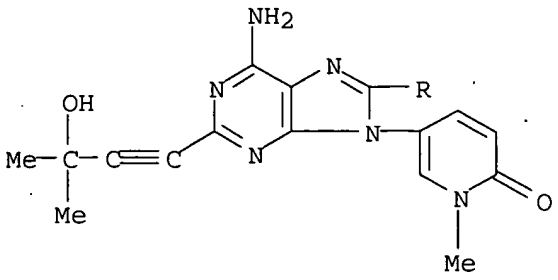
RN 318468-88-1 CAPLUS
CN 9H-Purin-6-amine, 9-(6-chloro-3-pyridazinyl)-8-(3-fluorophenyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)

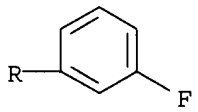


RN 318468-95-0 CAPLUS
CN 9H-Purin-6-amine, 8-(3-fluorophenyl)-9-(6-methoxy-3-pyridazinyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



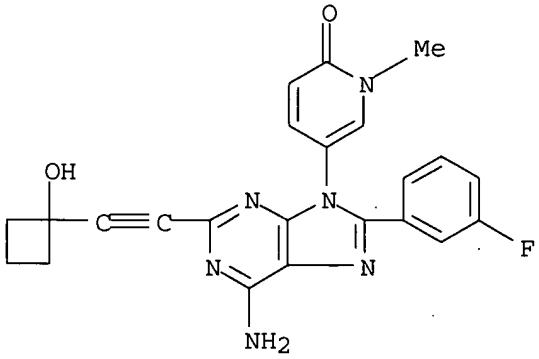
RN 318468-96-1 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-(3-hydroxy-3-methyl-1-butynyl)-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)





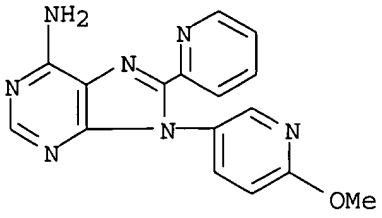
● HCl

RN 318468-97-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclobutyl)ethynyl]-9H-purin-9-yl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

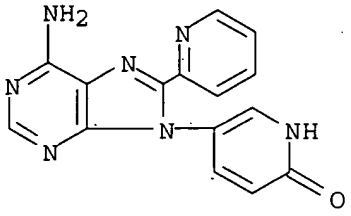


● HCl

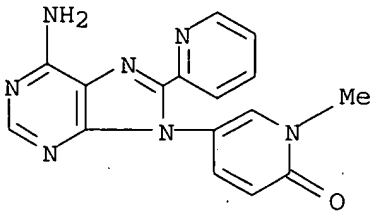
RN 318468-98-3 CAPLUS
CN 9H-Purin-6-amine, 9-(6-methoxy-3-pyridinyl)-8-(2-pyridinyl)- (9CI) (CA INDEX NAME)



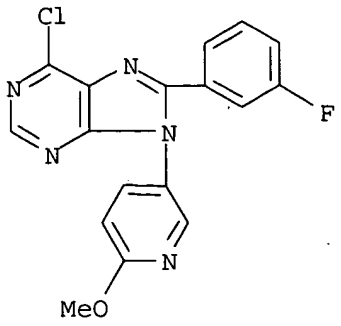
RN 318469-02-2 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(2-pyridinyl)-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



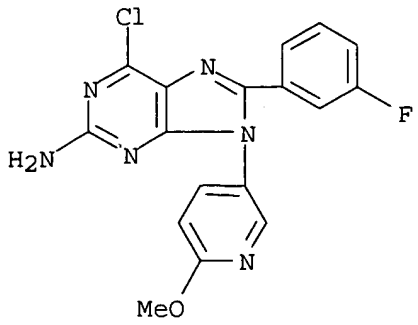
RN 318469-03-3 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-amino-8-(2-pyridinyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)



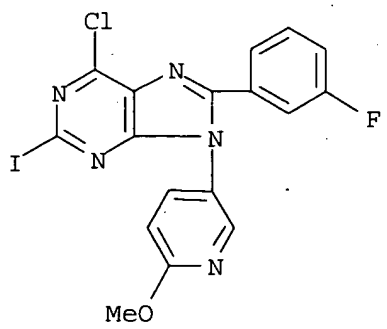
IT **318468-09-6P 318468-19-8P 318468-20-1P**
318468-54-1P 318468-76-7P 318468-82-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of fused imidazole compds. as antagonists of adenosine A2 receptors and remedies for diabetes mellitus)
RN 318468-09-6 CAPLUS
CN 9H-Purine, 6-chloro-8-(3-fluorophenyl)-9-(6-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



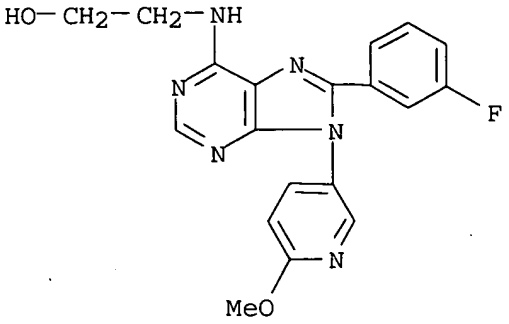
RN 318468-19-8 CAPLUS
CN 9H-Purin-2-amine, 6-chloro-8-(3-fluorophenyl)-9-(6-methoxy-3-pyridinyl)-(9CI) (CA INDEX NAME)



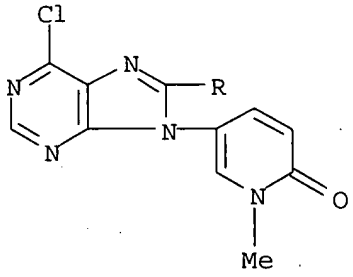
RN 318468-20-1 CAPLUS
CN 9H-Purine, 6-chloro-8-(3-fluorophenyl)-2-iodo-9-(6-methoxy-3-pyridinyl)-(9CI) (CA INDEX NAME)

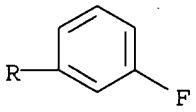


RN 318468-54-1 CAPLUS
CN Ethanol, 2-[[8-(3-fluorophenyl)-9-(6-methoxy-3-pyridinyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

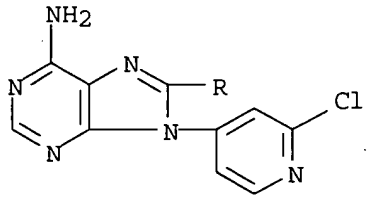


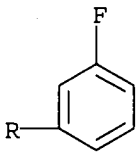
RN 318468-76-7 CAPLUS
CN 2(1H)-Pyridinone, 5-[6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl- (9CI) (CA INDEX NAME)



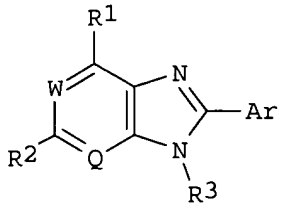


RN 318468-82-5 CAPLUS
CN 9H-Purin-6-amine, 9-(2-chloro-4-pyridinyl)-8-(3-fluorophenyl)- (9CI) (CA INDEX NAME)





GI



I

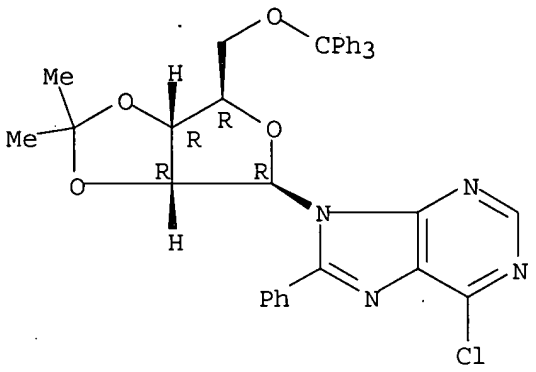
AB Novel fused imidazole compds. such as purine derivs. of general formula (I), pharmacol. acceptable salts thereof, or hydrates of both [wherein R1 = H, OH, halo, (un)substituted C1-8 alkyl, (un)substituted NH2; R2 = H, halo, (un)substituted NH2, (un)substituted C2-8 alkenyl, (un)substituted C3-8 alkynyl, (un)substituted C1-8 alkyl; R3 = (un)substituted C3-8 alkynyl, C3-8 alkenyl, (un)substituted C1-8 alkyl, (un)substituted aryl, (un)substituted heteroaryl, etc.; Ar = (un)substituted aryl, (un)substituted heteroaryl, optionally halo- or C1-6 alkyl-substituted N-C1-6 alkyl- or N-C3-6 cycloalkyl-oxopyridyl or -oxopyrimidyl; Q, W = N, CH; some proviso are given] are prepd. These compds. exhibit adenosine A2 receptor antagonism and are effective in the prevention and treatment of diabetes mellitus and complications of diabetes. Thus, 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1,2-dihydro-2-pyridinone was condensed with N,N-dimethylformamide di-Me acetal in DMF at room temp. for 1 h, ice-cooled, treated with NaH at 0-6.degree. for 30 min, and methylated by Me iodide at room temp. for 16 h to give 5-[6-amino-8-(3-fluorophenyl)-9H-purin-9-yl]-1-methyl-1,2-dihydro-2-pyridinone (II). II.HCl at 10 mg/kg p.o. in spontaneously diabetic mice lowered the blood sugar level to 47.3.+-.7.2% of the control animal.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1999:629465 CAPLUS
DN 131:337302
TI First Evident Generation of Purin-2-yllithium: Lithiation of an 8-Silyl-Protected 6-Chloropurine Riboside as a Key Step for the Synthesis of 2-Carbon-Substituted Adenosines
AU Kumamoto, Hiroki; Tanaka, Hiromichi; Tsukioka, Ryota; Ishida, Yumiko; Nakamura, Akiko; Kimura, Satoe; Hayakawa, Hiroyuki; Kato, Keisuke; Miyasaka, Tadashi
CS School of Pharmaceutical Sciences, Showa University, Shinagawa-ku Tokyo, 142-8555, Japan
SO Journal of Organic Chemistry (1999), 64(21), 7773-7780
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:337302
IT **249757-31-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(first evident generation of purinyl-lithium via lithiation of a silyl-protected chloropurine riboside as a key step)

RN 249757-31-1 CAPLUS
CN 9H-Purine, 6-chloro-9-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.beta.-D-ribofuranosyl]-8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Lithiation at the 2-position of a purine ring has been accomplished for the first time by using 6-chloro-9-(2,3-O-isopropylidene-5-O-trityl-.beta.-D-ribofuranosyl)-8-(triisopropylsilyl)purine as a substrate and LTMP as a lithiating agent. The 8-triisopropylsilyl group did not undergo anionic migration and, thus, allowed the ready generation of the C2-lithiated species by preventing deprotonation at the 8-position. The electron-withdrawing 6-chlorine atom plays an essential role to this C2-lithiation. Reactions of the lithiated species with electrophiles gave the 2-substituted products (Me, Et, i-Pr, CH(OH)C6H11, C(OH)Me2, CHO, CO2Me, and I) mostly in good yields. Ammonolysis of the 6-chlorine atom of these products (heating at 110 .degree.C in a sealed tube with NH3/MeOH) effected simultaneous desilylation at the 8-position to give the corresponding adenosine analogs. The whole sequence provides a new and highly general method for the synthesis of 2-substituted adenosines.
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1999:451298 CAPLUS
DN 131:116251
TI Preparation of purine derivatives as adenosine A2 receptor antagonists for the treatment of diabetes
IN Asano, Osamu; Harada, Hitoshi; Hoshino, Yorihisa; Yoshikawa, Seiji; Inoue, Takashi; Horizoe, Tatsuo; Yasuda, Nobuyuki; Nagata, Kaya; Nagaoka, Junsaku; Murakami, Manabu; Kobayashi, Seiichi
PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 167 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9935147	A1	19990715	WO 1998-JP5870	19981224

W: AU, BR, CA, CN, HU, KR, MX, NO, NZ, RU, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

			JP 1998-526	A 19980105
JP 11263789	A2	19990928	JP 1998-363938	19981222
			JP 1998-526	A 19980105
CA 2315736	AA	19990715	CA 1998-2315736	19981224
			JP 1998-526	A 19980105
			WO 1998-JP5870	W 19981224
AU 9916885	A1	19990726	AU 1999-16885	19981224
			JP 1998-526.	A 19980105
			WO 1998-JP5870	W 19981224
EP 1054012	A1	20001122	EP 1998-961528	19981224
EP 1054012	B1	20030611		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
			JP 1998-526	A 19980105
			WO 1998-JP5870	W 19981224
EP 1300147	A1	20030409	EP 2002-29118	19981224
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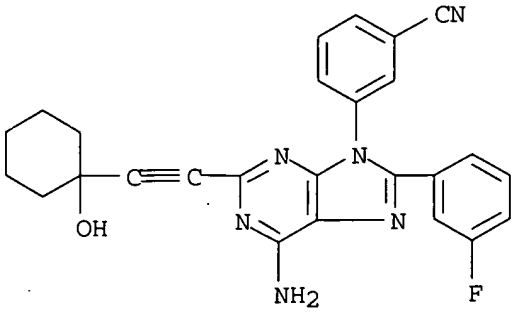
			JP 1998-526	A 19980105
			EP 1998-961528	A3 19981224
US 6579868	B1	20030617	US 2000-582840	20000705
			JP 1998-526	A 19980105
			WO 1998-JP5870	W 19981224

OS MARPAT 131:116251

IT **232252-44-7P 232252-45-8P 232252-46-9P**
232252-47-0P 232252-48-1P 232252-49-2P
232252-50-5P 232252-54-9P 232252-55-0P
232252-56-1P 232252-57-2P 232252-58-3P
232252-59-4P 232252-60-7P 232252-61-8P
232252-62-9P 232253-00-8P 232253-03-1P
232253-54-2P 232253-56-4P 232253-87-1P
232253-88-2P 232254-05-6P 232254-66-9P
232254-72-7P 232254-73-8P 232254-74-9P
232254-75-0P 232254-86-3P 232255-16-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of purine derivs. as adenosine A2 receptor antagonists for treatment of diabetes)

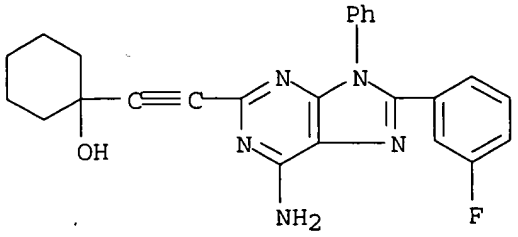
RN 232252-44-7 CAPLUS

CN Benzonitrile, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



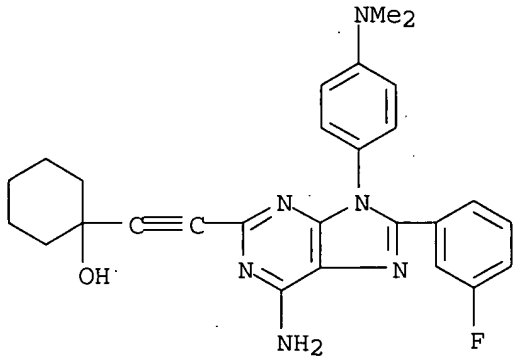
RN 232252-45-8 CAPLUS

CN Cyclohexanol, 1-[[6-amino-8-(3-fluorophenyl)-9-phenyl-9H-purin-2-yl]ethynyl]-, monohydrochloride (9CI) (CA INDEX NAME)



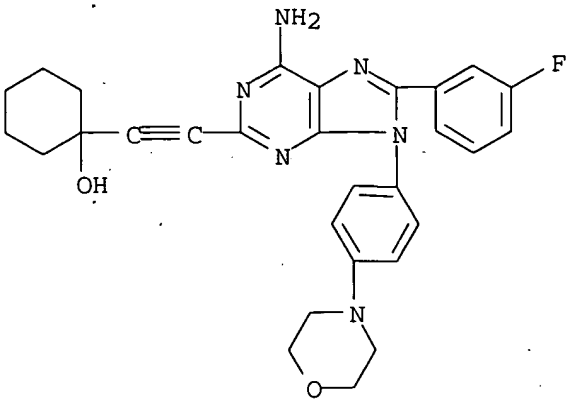
● HCl

RN 232252-46-9 CAPLUS
CN Cyclohexanol, 1-[[6-amino-9-[4-(dimethylamino)phenyl]-8-(3-fluorophenyl)-9H-purin-2-yl]ethynyl]-, dihydrochloride (9CI) (CA INDEX NAME)



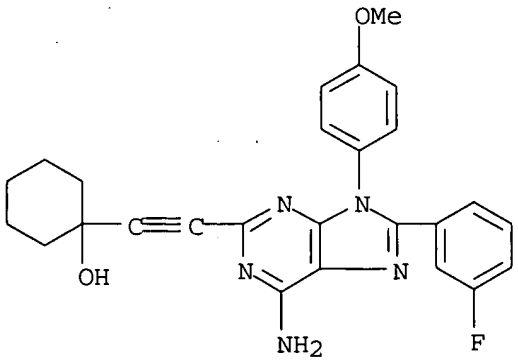
●2 HCl

RN 232252-47-0 CAPLUS
CN Cyclohexanol, 1-[[6-amino-8-(3-fluorophenyl)-9-[4-(4-morpholinyl)phenyl]-9H-purin-2-yl]ethynyl]-, dihydrochloride (9CI) (CA INDEX NAME)



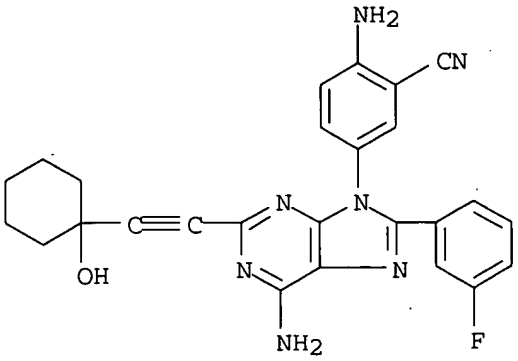
● 2 HCl

RN 232252-48-1 CAPLUS
CN Cyclohexanol, 1-[[6-amino-8-(3-fluorophenyl)-9-(4-methoxyphenyl)-9H-purin-2-yl]ethynyl]-, monohydrochloride (9CI) (CA INDEX NAME)



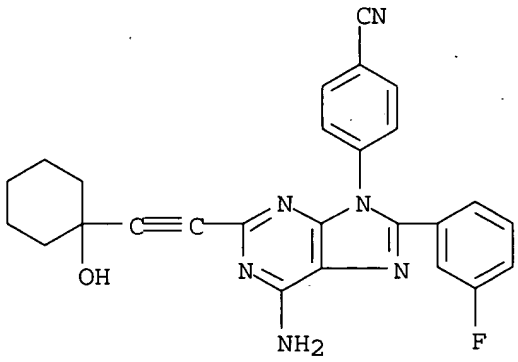
● HCl

RN 232252-49-2 CAPLUS
CN Benzonitrile, 2-amino-5-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, dihydrochloride (9CI) (CA INDEX NAME)



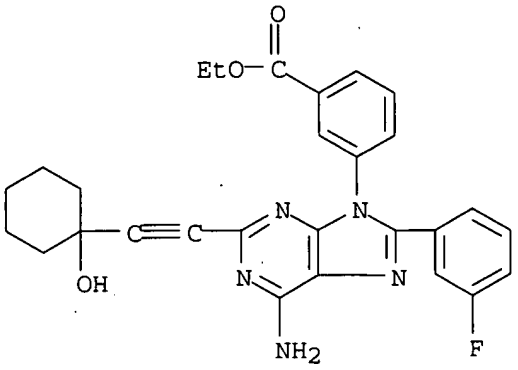
● 2 HCl

RN 232252-50-5 CAPLUS
CN Benzonitrile, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



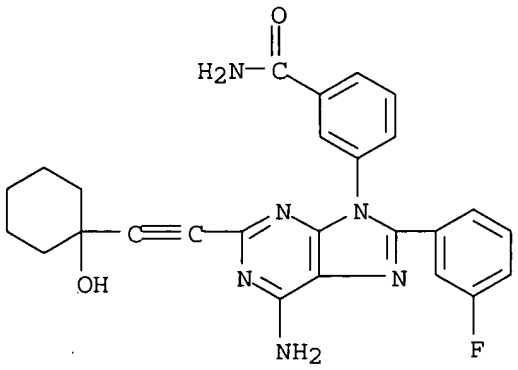
● HCl

RN 232252-54-9 CAPLUS
CN Benzoic acid, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

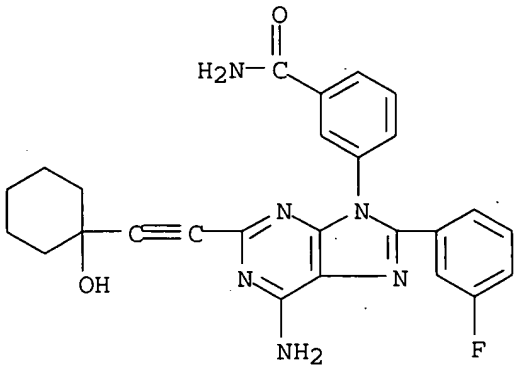


● HCl

RN 232252-55-0 CAPLUS
CN Benzamide, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)

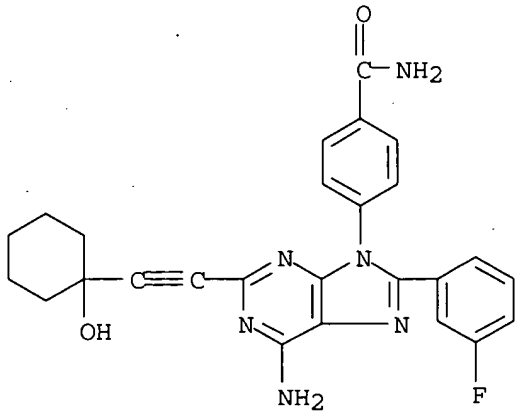


RN 232252-56-1 CAPLUS
CN Benzamide, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



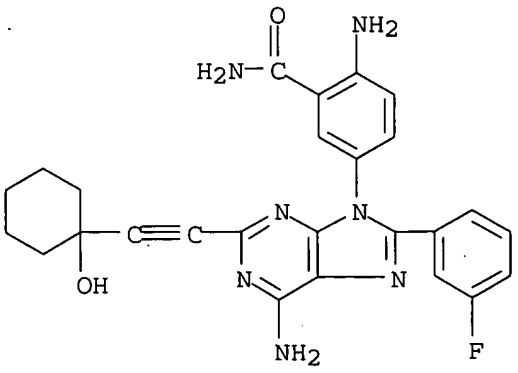
● HCl

RN 232252-57-2 CAPLUS
CN Benzamide, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



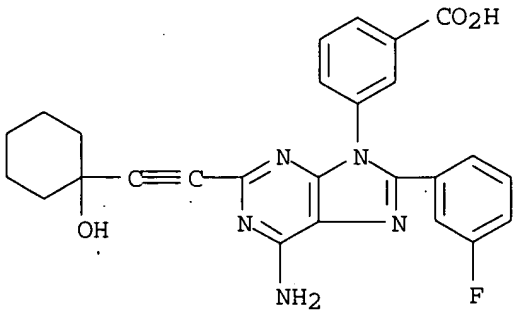
● HCl

RN 232252-58-3 CAPLUS
CN Benzamide, 2-amino-5-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, dihydrochloride (9CI) (CA INDEX NAME)



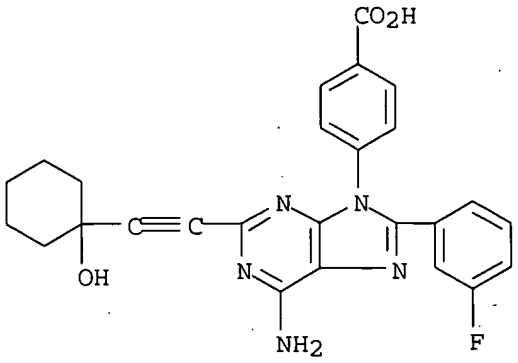
● 2 HCl

RN 232252-59-4 CAPLUS
CN Benzoic acid, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



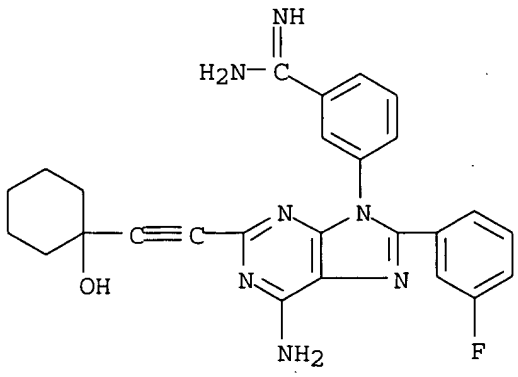
● HCl

RN 232252-60-7 CAPLUS
CN Benzoic acid, 4-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



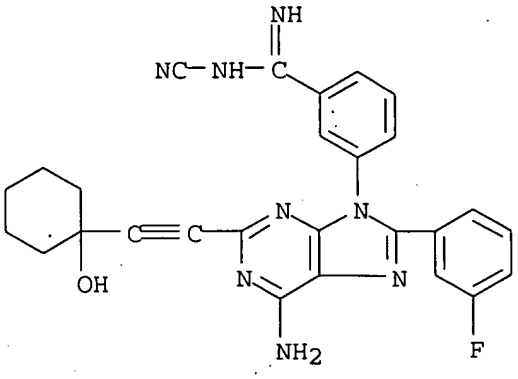
● HCl

RN 232252-61-8 CAPLUS
CN Benzenecarboximidamide, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-, dihydrochloride (9CI) (CA INDEX NAME)



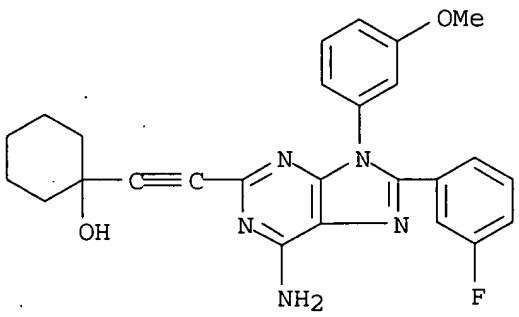
●2 HCl

RN 232252-62-9 CAPLUS
CN Benzenecarboximidamide, 3-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]-N-cyano-, dihydrochloride (9CI) (CA INDEX NAME)



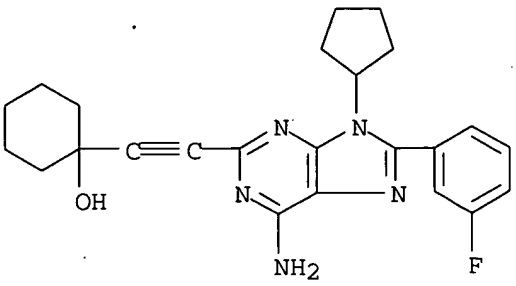
● 2 HCl

RN 232253-00-8 CAPLUS
CN Cyclohexanol, 1-[[6-amino-8-(3-fluorophenyl)-9-(3-methoxyphenyl)-9H-purin-2-yl]ethynyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

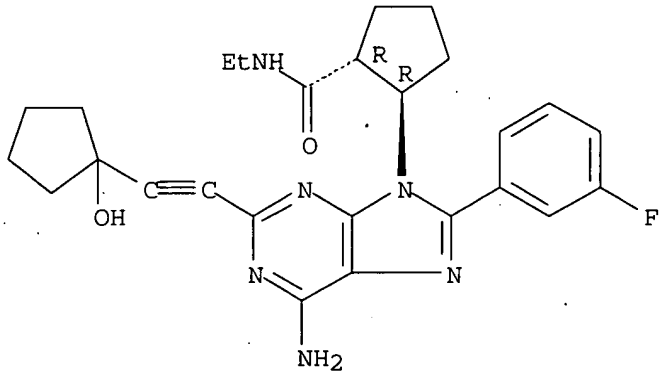
RN 232253-03-1 CAPLUS
CN Cyclohexanol, 1-[[6-amino-9-cyclopentyl-8-(3-fluorophenyl)-9H-purin-2-yl]ethynyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

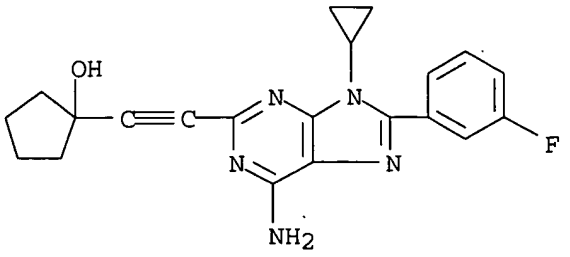
RN 232253-54-2 CAPLUS
CN Cyclopentanecarboxamide, 2-[6-amino-8-(3-fluorophenyl)-2-[(1-hydroxycyclopentyl)ethynyl]-9H-purin-9-yl]-N-ethyl-, monohydrochloride, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



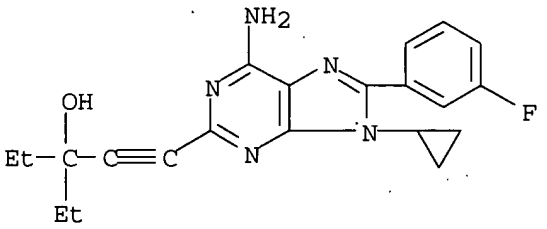
● HCl

RN 232253-56-4 CAPLUS
CN Cyclopentanol, 1-[[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]ethynyl]-, monohydrochloride (9CI) (CA INDEX NAME)



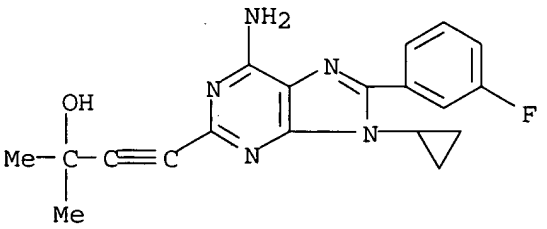
● HCl

RN 232253-87-1 CAPLUS
CN 1-Pentyn-3-ol, 1-[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]-3-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



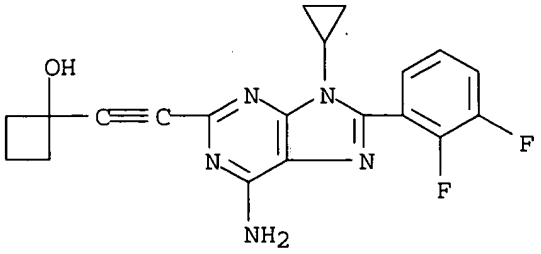
● HCl

RN 232253-88-2 CAPLUS
CN 3-Butyn-2-ol, 4-[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

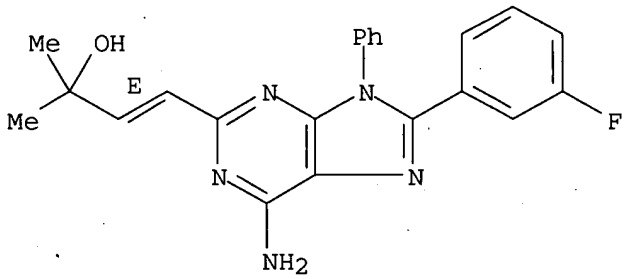
RN 232254-05-6 CAPLUS
CN Cyclobutanol, 1-[[6-amino-9-cyclopropyl-8-(2,3-difluorophenyl)-9H-purin-2-yl]ethynyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 232254-66-9 CAPLUS
CN 3-Buten-2-ol, 4-[6-amino-8-(3-fluorophenyl)-9-phenyl-9H-purin-2-yl]-2-methyl-, monohydrochloride, (3E)- (9CI) (CA INDEX NAME)

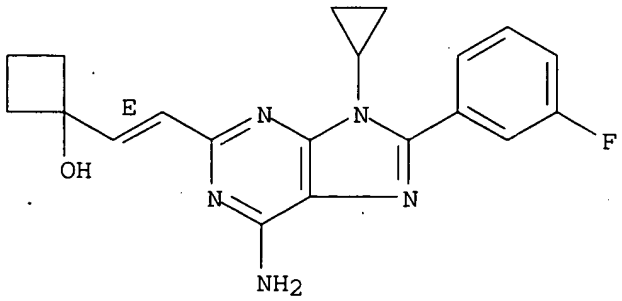
Double bond geometry as shown.



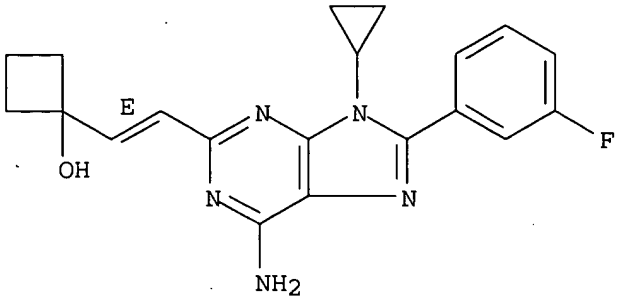
● HCl

RN 232254-72-7 CAPLUS
CN Cyclobutanol, 1-[(1E)-2-[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]ethenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.



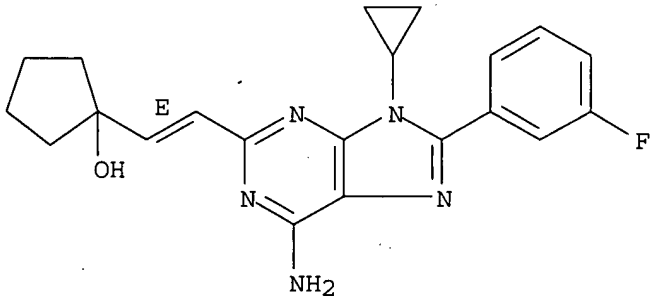
● HCl



● HCl

RN 232254-73-8 CAPLUS
CN Cyclopentanol, 1-[(1E)-2-[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]ethenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

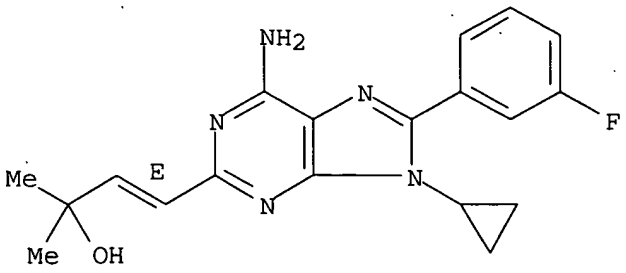
Double bond geometry as shown.



● HCl

RN 232254-74-9 CAPLUS
CN 3-Buten-2-ol, 4-[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]-2-methyl-, monohydrochloride, (3E)- (9CI) (CA INDEX NAME)

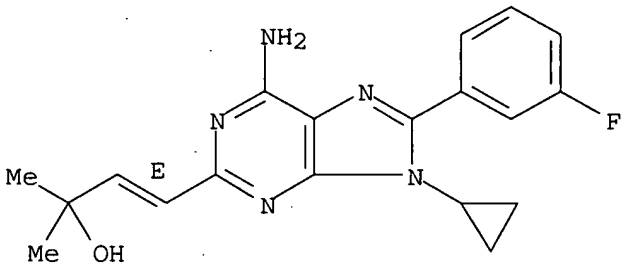
Double bond geometry as shown.



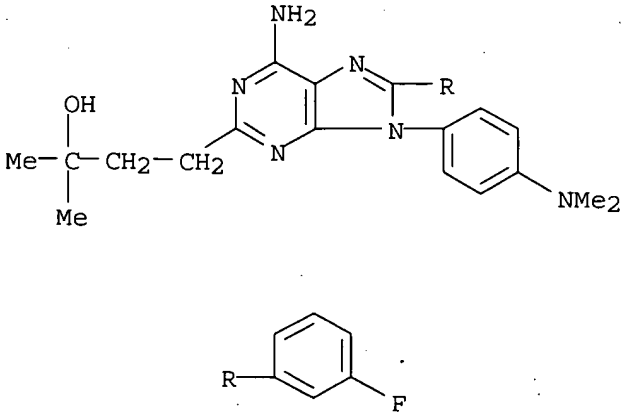
● HCl

RN 232254-75-0 CAPLUS
CN 3-Buten-2-ol, 4-[6-amino-9-cyclopropyl-8-(3-fluorophenyl)-9H-purin-2-yl]-2-methyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

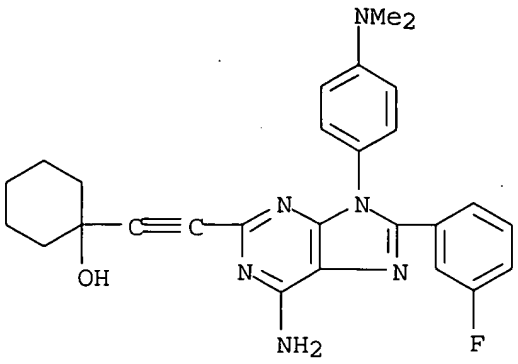


RN 232254-86-3 CAPLUS
CN 9H-Purine-2-propanol, 6-amino-9-[4-(dimethylamino)phenyl]-8-(3-fluorophenyl)-.alpha.,.alpha.-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



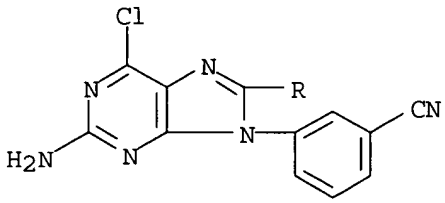
●2 HCl

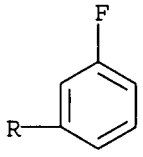
RN 232255-16-2 CAPLUS
CN Cyclohexanol, 1-[[6-amino-9-[4-(dimethylamino)phenyl]-8-(3-fluorophenyl)-9H-purin-2-yl]ethynyl]- (9CI) (CA INDEX NAME)



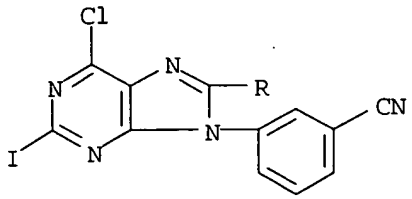
IT **232254-90-9P 232254-91-0P 232254-92-1P**
232254-93-2P 232254-94-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of purine derivs. as adenosine A2 receptor antagonists for treatment of diabetes)

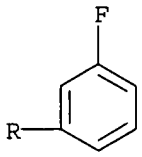
RN 232254-90-9 CAPLUS
CN Benzonitrile, 3-[2-amino-6-chloro-8-(3-fluorophenyl)-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



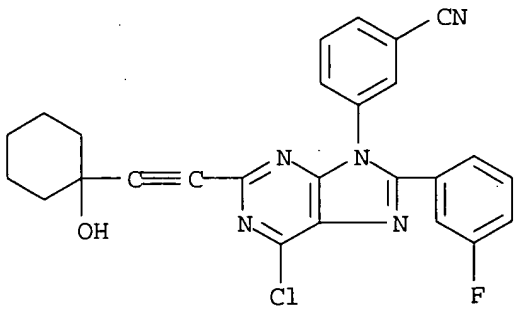


RN 232254-91-0 CAPLUS
CN Benzonitrile, 3-[6-chloro-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]- (9CI) (CA INDEX NAME)

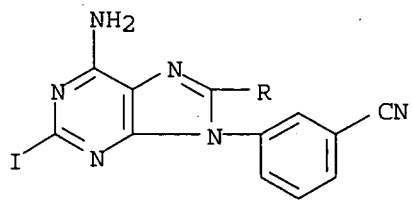


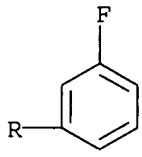


RN 232254-92-1 CAPLUS
CN Benzonitrile, 3-[6-chloro-8-(3-fluorophenyl)-2-[(1-hydroxycyclohexyl)ethynyl]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



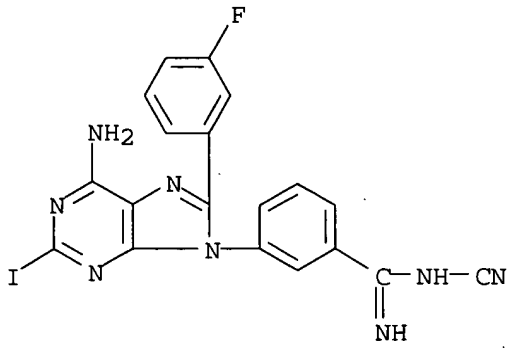
RN 232254-93-2 CAPLUS
CN Benzonitrile, 3-[6-amino-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



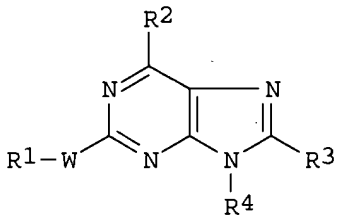


RN 232254-94-3 CAPLUS

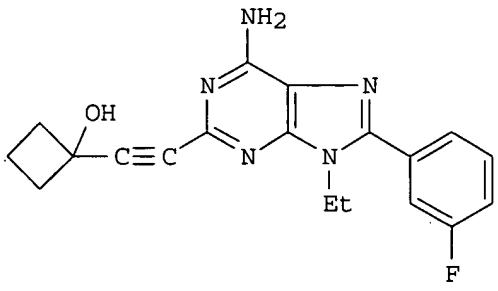
CN Benzenecarboximidamide, 3-[6-amino-8-(3-fluorophenyl)-2-iodo-9H-purin-9-yl]-N-cyano- (9CI) (CA INDEX NAME)



GI



I



II

AB The title compds. I [R1 = (un)substituted arom. ring (which may contain heteroatom), etc.; W = CH2CH2, etc.; R2 = H, (un)substituted alkyl, etc.; R3 = H, (un)substituted cycloalkyl, etc.; R4 = H, (un)substituted alkyl, heteroaryl, etc.; a proviso is given] are prepd. In an in vitro test for A2a receptor antagonism, the title compd. II showed the Ki value of 0.002 .mu.M.

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1999:112311 CAPLUS
DN 130:209672
TI Synthesis, corticotropin-releasing factor receptor binding affinity, and

pharmacokinetic properties of triazolo-, imidazo-, and pyrrolopyrimidines and -pyridines

AU Chorvat, Robert J.; Bakthavatchalam, Rajagopal; Beck, James P.; Gilligan, Paul J.; Wilde, Richard G.; Cocuzza, Anthony J.; Hobbs, Frank W.; Cheeseman, Robert S.; Curry, Matthew; Rescinito, Joseph P.; Krenitsky, Paul; Chidester, Dennis; Yarem, Jerry A.; Klaczkiewicz, John D.; Hodge, C. Nicholas; Aldrich, Paul E.; Wasserman, Zelda R.; Fernandez, Christine H.; Zaczek, Robert; Fitzgerald, Lawrence W.; Huang, Shiew-Mei; Shen, Helen L.; Wong, Y. Nancy; Chien, Ben M.; Quon, Check Y.; Arvanitis, Argyrios

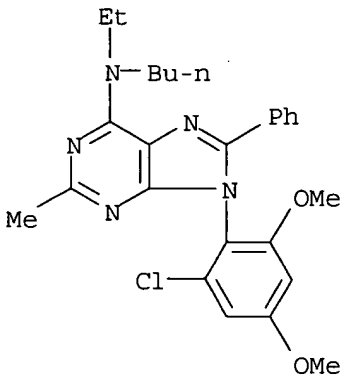
CS Departments of Chemical and Physical Sciences and of Biological Sciences, DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA

SO Journal of Medicinal Chemistry (1999), 42(5), 833-848
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English

IT **220953-13-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(CRF receptor binding affinity of triazolo-, imidazo-, and pyrrolopyrimidines and -pyridines prepd. from amines, alcs., pyrimidine and pyridine derivs.)

RN 220953-13-9 CAPLUS

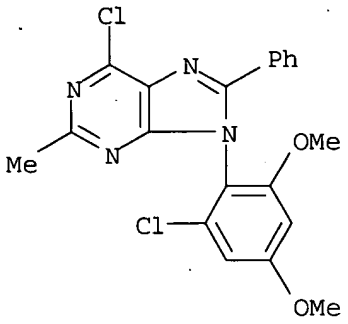
CN 9H-Purin-6-amine, N-butyl-9-(2-chloro-4,6-dimethoxyphenyl)-N-ethyl-2-methyl-8-phenyl- (9CI) (CA INDEX NAME)



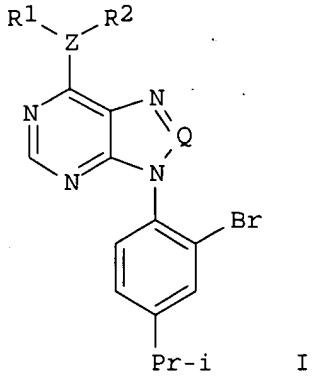
IT **220952-86-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(CRF receptor binding affinity of triazolo-, imidazo-, and pyrrolopyrimidines and -pyridines prepd. from amines, alcs., pyrimidine and pyridine derivs.)

RN 220952-86-3 CAPLUS

CN 9H-Purine, 6-chloro-9-(2-chloro-4,6-dimethoxyphenyl)-2-methyl-8-phenyl- (9CI) (CA INDEX NAME)



GI



I

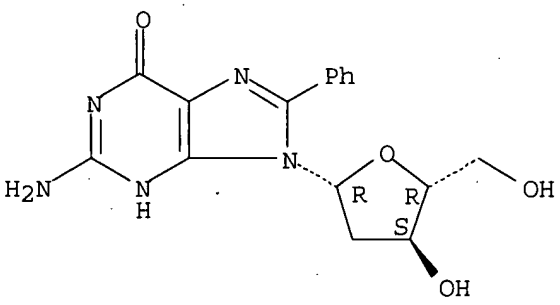
AB The synthesis and CRF receptor binding affinities of several new series of N-aryltriazolo- and -imidazopyrimidines and -pyridines, e.g., I (R1 = n-Bu, CHEt2, CHEtCH2OH, etc., R2 = Et, H, Me, etc., Q = N, CH, CMe, CCF3, Z = N, O), are described. These cyclized systems were prepd. from appropriately substituted diaminopyrimidines or -pyridines by nitrous acid, orthoester, or acyl halide treatment. Variations of amino (ether) pendants and arom. substituents have defined the structure-activity relationships of these series and resulted in the identification of a variety of high-affinity agents (Ki's < 10 nM). On the basis of this property and lipophilicity differences, six of these compds. were initially chosen for rat pharmacokinetic (PK) studies. Good oral bioavailability, high plasma levels, and duration of four of these compds. prompted further PK studies in the dog following both i.v. and oral routes of administration. Results from this work indicated I [R1 = R2 = (CH2)OMe, Q = Z = N; R1 CHEtCH2OMe, R2 = H, Q = Z = N] had properties believe to be necessary for a potential therapeutic agent, and I [R1 = R2 = (CH2)OMe, Q = Z = N] has been selected for further pharmacol. studies that will be reported in due course.

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1997:757616 CAPLUS
DN 128:58662

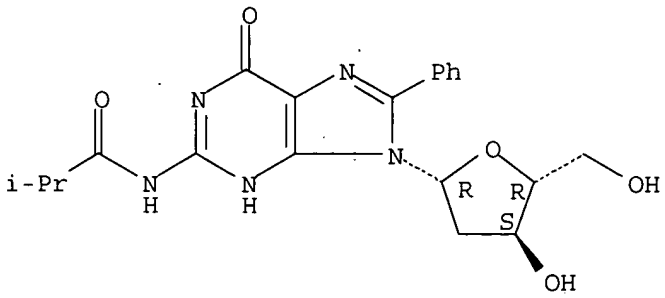
TI Synthesis and Miscoding Specificity of Oligodeoxynucleotide Containing 8-Phenyl-2'-deoxyguanosine
AU Kohda, Kohfuku; Tsunomoto, Hirotaka; Kasamatsu, Toshio; Sawamura, Fumiko; Terashima, Isamu; Shibutani, Shinya
CS Faculty of Pharmaceutical Sciences, Nagoya City University, Nagoya, 467, Japan
SO Chemical Research in Toxicology (1997), 10(12), 1351-1358
CODEN: CRTOEC; ISSN: 0893-228X
PB American Chemical Society
DT Journal
LA English
OS CASREACT 128:58662
IT **199991-98-5P 199992-01-3P 199992-04-6P**
199992-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and miscoding specificity of oligodeoxynucleotide contg. 8-phenyl-2'-deoxyguanosine)
RN 199991-98-5 CAPLUS
CN Guanosine, 2'-deoxy-8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



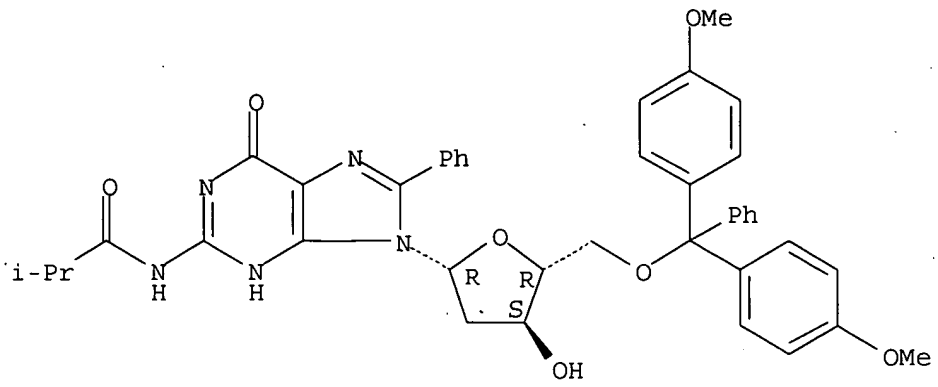
RN 199992-01-3 CAPLUS
CN Guanosine, 2'-deoxy-N-(2-methyl-1-oxopropyl)-8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



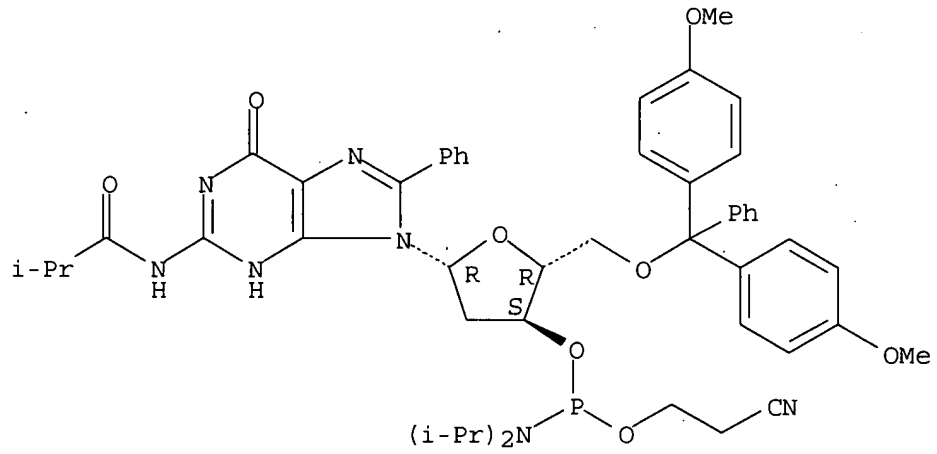
RN 199992-04-6 CAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-N-(2-methyl-1-oxopropyl)-8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 199992-07-9 CAPLUS
CN Guanosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-N-(2-methyl-1-oxopropyl)-8-phenyl-, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Aryl radicals and arenediazonium ions are suspected to react with cellular DNA, resulting in C8-arylguanine adducts. 8-Phenyl-2'-deoxyguanosine (8-PhdG) was synthesized as a model adduct by reacting dG with benzenediazonium chloride and incorporated into oligodeoxynucleotides using phosphoramidite techniques. A site-specifically modified oligodeoxynucleotide contg. a single 8-PhdG was then used as a template for primer extension reactions catalyzed by the intact (exo+) or 3'.fwdarw.5' exonuclease-free (exo-) Klenow fragment of Escherichia coli DNA polymerase I and mammalian DNA polymerase a (pol .alpha.). Although primer extensions catalyzed by the Klenow fragments were retarded at the position of 8-PhdG, most of the primer extension passed the lesion to form the fully extended products. In contrast, primer extensions catalyzed by pol .alpha. were strongly blocked opposite the lesion. The fully extended products formed during DNA synthesis were analyzed to quantify the miscoding specificities of 8-PhdG. The exo- Klenow fragment incorporated primarily dCMP, the correct base, opposite 8-PhdG, along with small amts. of incorporation of dAMP. Two-base deletions were also obsd. In

contrast, the exo+ Klenow fragment incorporated dCMP opposite the lesion. When pol .alpha. was used, 8-PhdG promoted small amts. of misincorporation of dAMP and dGMP as well as one- and two-base deletions. The duplex contg. 8-PhdG.cntdot.dG was thermally and thermodynamically more stable than dG.cntdot.dG. The duplex contg. 8-PhdG.cntdot.dA was thermodynamically more stable than dG.cntdot.dA. We conclude that 8-PhdG is a weak miscoding lesion, capable of generating G .fwdarw. T and G .fwdarw. C transversions and deletions in cells.

L4 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1997:15548 CAPLUS
DN 126:104368
TI Process for the preparation of purine nucleosides using palladium-catalyzed coupling reaction
IN Tu, Chi; Eaton, Bruce
PA Nexstar Pharmaceuticals, Inc., USA
SO U.S., 7 pp., Cont.-in-part of U.S. 5,428,149.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5580972	A	19961203	US 1994-347600	19941201
				US 1993-76735 A2	19930614
	US 5428149	A	19950627	US 1993-76735	19930614
	CA 2164935	AA	19941222	CA 1994-2164935	19940531
				US 1993-76735 A	19930614
	US 5633361	A	19970527	US 1995-407893	19950321
				US 1993-76735 A3	19930614
	US 5591843	A	19970107	US 1995-423395	19950419
				US 1993-76735 A3	19930614
	US 5783679	A	19980721	US 1995-441881	19950516
				US 1993-76735 A2	19930614
				US 1994-347600 A1	19941201
	WO 9616972	A1	19960606	WO 1995-US15124	19951120
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1994-347600 A	19941201
	AU 9642412	A1	19960619	AU 1996-42412	19951120
				US 1994-347600 A	19941201
				WO 1995-US15124W	19951120

PATENT FAMILY INFORMATION:
FAN 1995:422814

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9429279	A1	19941222	WO 1994-US5946	19940531
	W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1993-76735 A	19930614

	US 5428149	A	19950627	US 1993-76735	19930614
	CA 2164935	AA	19941222	CA 1994-2164935	19940531
				US 1993-76735 A	19930614
	AU 9470461	A1	19950103	AU 1994-70461	19940531
	AU 683665	B2	19971120		
				US 1993-76735 A	19930614
				WO 1994-US5946 W	19940531
	EP 702675	A1	19960327	EP 1994-919254	19940531
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
				US 1993-76735 A	19930614
				WO 1994-US5946 W	19940531
	JP 08511527	T2	19961203	JP 1994-501854	19940531
				US 1993-76735 A	19930614
				WO 1994-US5946 W	19940531
	US 5633361	A	19970527	US 1995-407893	19950321
				US 1993-76735 A319930614	
	US 5591843	A	19970107	US 1995-423395	19950419
				US 1993-76735 A319930614	

FAN 1996:476827

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9616972	A1	19960606	WO 1995-US15124	19951120
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1994-347600 A	19941201
	US 5580972	A	19961203	US 1994-347600	19941201
				US 1993-76735 A219930614	
	AU 9642412	A1	19960619	AU 1996-42412	19951120
				US 1994-347600 A	19941201
				WO 1995-US15124W	19951120

FAN 1997:88785

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9638460	A1	19961205	WO 1996-US8026	19960530
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
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				US 1995-458421 A	19950602
				US 1995-459073 A	19950602
	US 5719273	A	19980217	US 1995-458421	19950602
				US 1993-76735 A219930614	
	AU 9661468	A1	19961218	AU 1996-61468	19960530
	AU 721747	B2	20000713		
				US 1995-458421 A	19950602
				US 1995-459073 A	19950602
				WO 1996-US8026 W	19960530
	EP 828750	A1	19980318	EP 1996-919015	19960530
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
				US 1995-458421 A	19950602

				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	JP 11506107	T2	19990602	JP 1996-536652 19960530
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	US 5945527	A	19990831	US 1997-952338 19971104
				WO 1996-US8026 W 19960530

FAN 1998:149514

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5719273	A	19980217	US 1995-458421	19950602
				US 1993-76735	A219930614
	US 5428149	A	19950627	US 1993-76735	19930614
	CA 2164935	AA	19941222	CA 1994-2164935	19940531
				US 1993-76735	A 19930614
	US 5633361	A	19970527	US 1995-407893	19950321
				US 1993-76735	A319930614
	US 5591843	A	19970107	US 1995-423395	19950419
				US 1993-76735	A319930614
	CA 2221279	AA	19961205	CA 1996-2221279	19960530
				US 1995-458421	A 19950602
				US 1995-459073	A 19950602
	WO 9638460	A1	19961205	WO 1996-US8026	19960530
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
				US 1995-458421	A 19950602
				US 1995-459073	A 19950602
	AU 9661468	A1	19961218	AU 1996-61468	19960530
	AU 721747	B2	20000713		
				US 1995-458421	A 19950602
				US 1995-459073	A 19950602
				WO 1996-US8026	W 19960530
	EP 828750	A1	19980318	EP 1996-919015	19960530
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
				US 1995-458421	A 19950602
				US 1995-459073	A 19950602
				WO 1996-US8026	W 19960530
	JP 11506107	T2	19990602	JP 1996-536652	19960530
				US 1995-458421	A 19950602
				US 1995-459073	A 19950602
				WO 1996-US8026	W 19960530

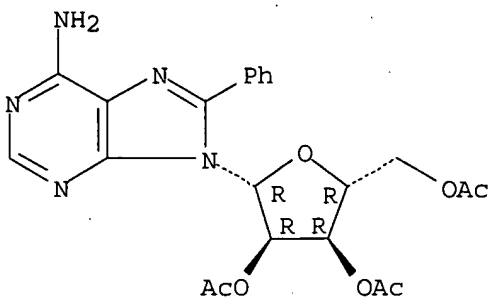
OS CASREACT 126:104368; MARPAT 126:104368

IT **172945-44-7P 172945-47-0P 172945-50-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the prepn. of purine nucleosides using palladium-catalyzed coupling reaction)

RN 172945-44-7 CAPLUS

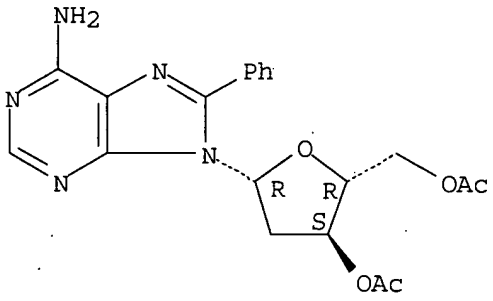
CN Adenosine, 8-phenyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



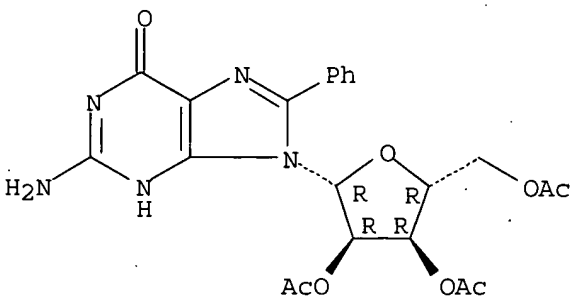
RN 172945-47-0 CAPLUS
CN Adenosine, 2'-deoxy-8-phenyl-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

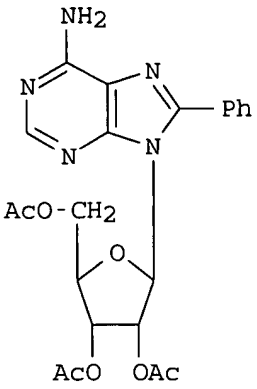


RN 172945-50-5 CAPLUS
CN Guanosine, 8-phenyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



I

AB Improved method for the prepn. of modified purine nucleosides at the 2-, 6-, or 8-position of the purine ring, e.g. I, using a palladium-catalyzed coupling reaction, is reported.

L4 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1996:476827 CAPLUS
DN 125:143238
TI Palladium-catalyzed C-alkenylation of purine nucleosides with organotins
IN Tu, Chi; Eaton, Bruce
PA Nexstar Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9616972	A1	19960606	WO 1995-US15124	19951120
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1994-347600 A	19941201
	US 5580972	A	19961203	US 1994-347600	19941201
				US 1993-76735 A2	19930614
	AU 9642412	A1	19960619	AU 1996-42412	19951120
				US 1994-347600 A	19941201
				WO 1995-US15124W	19951120

PATENT FAMILY INFORMATION:
FAN 1995:422814

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9429279	A1	19941222	WO 1994-US5946	19940531
	W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1993-76735 A	19930614

	US 5428149	A	19950627	US 1993-76735	19930614
	CA 2164935	AA	19941222	CA 1994-2164935	19940531
				US 1993-76735 A	19930614
	AU 9470461	A1	19950103	AU 1994-70461	19940531
	AU 683665	B2	19971120		
				US 1993-76735 A	19930614
				WO 1994-US5946 W	19940531
	EP 702675	A1	19960327	EP 1994-919254	19940531
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
				US 1993-76735 A	19930614
				WO 1994-US5946 W	19940531
	JP 08511527	T2	19961203	JP 1994-501854	19940531
				US 1993-76735 A	19930614
				WO 1994-US5946 W	19940531
	US 5633361	A	19970527	US 1995-407893	19950321
				US 1993-76735 A	319930614
	US 5591843	A	19970107	US 1995-423395	19950419
				US 1993-76735 A	319930614

FAN 1997:15548

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5580972	A	19961203	US 1994-347600	19941201
				US 1993-76735 A	219930614
	US 5428149	A	19950627	US 1993-76735	19930614
	CA 2164935	AA	19941222	CA 1994-2164935	19940531
				US 1993-76735 A	19930614
	US 5633361	A	19970527	US 1995-407893	19950321
				US 1993-76735 A	319930614
	US 5591843	A	19970107	US 1995-423395	19950419
				US 1993-76735 A	319930614
	US 5783679	A	19980721	US 1995-441881	19950516
				US 1993-76735 A	219930614
				US 1994-347600 A	119941201
	WO 9616972	A1	19960606	WO 1995-US15124	19951120
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				US 1994-347600 A	19941201
	AU 9642412	A1	19960619	AU 1996-42412	19951120
				US 1994-347600 A	19941201
				WO 1995-US15124W	19951120

FAN 1997:88785

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9638460	A1	19961205	WO 1996-US8026	19960530
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
				US 1995-458421 A	19950602
				US 1995-459073 A	19950602
	US 5719273	A	19980217	US 1995-458421	19950602

				US 1993-76735 A219930614
	AU 9661468	A1	19961218	AU 1996-61468 19960530
	AU 721747	B2	20000713	
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	EP 828750	A1	19980318	EP 1996-919015 19960530
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	JP 11506107	T2	19990602	JP 1996-536652 19960530
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	US 5945527	A	19990831	US 1997-952338 19971104
				WO 1996-US8026 W 19960530

FAN 1998:149514

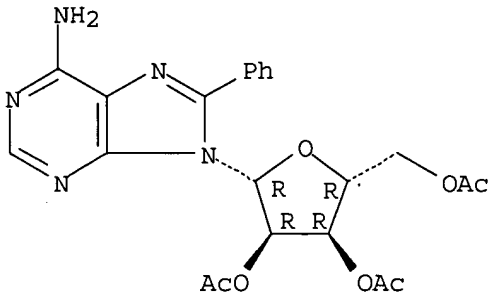
	PATENT NO.	KIND	DATE	APPLICATION NO. DATE
PI	US 5719273	A	19980217	US 1995-458421 19950602
				US 1993-76735 A219930614
	US 5428149	A	19950627	US 1993-76735 19930614
	CA 2164935	AA	19941222	CA 1994-2164935 19940531
				US 1993-76735 A 19930614
	US 5633361	A	19970527	US 1995-407893 19950321
				US 1993-76735 A319930614
	US 5591843	A	19970107	US 1995-423395 19950419
				US 1993-76735 A319930614
	CA 2221279	AA	19961205	CA 1996-2221279 19960530
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
	WO 9638460	A1	19961205	WO 1996-US8026 19960530
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI			
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA			
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
	AU 9661468	A1	19961218	AU 1996-61468 19960530
	AU 721747	B2	20000713	
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	EP 828750	A1	19980318	EP 1996-919015 19960530
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530
	JP 11506107	T2	19990602	JP 1996-536652 19960530
				US 1995-458421 A 19950602
				US 1995-459073 A 19950602
				WO 1996-US8026 W 19960530

OS CASREACT 125:143238; MARPAT 125:143238

IT **172945-44-7P 172945-47-0P 172945-50-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(palladium-catalyzed C-alkenylation of purine nucleosides with organotins)

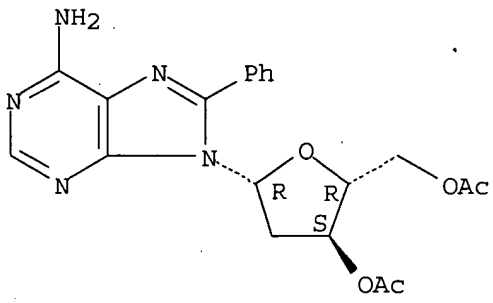
RN 172945-44-7 CAPLUS
CN Adenosine, 8-phenyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



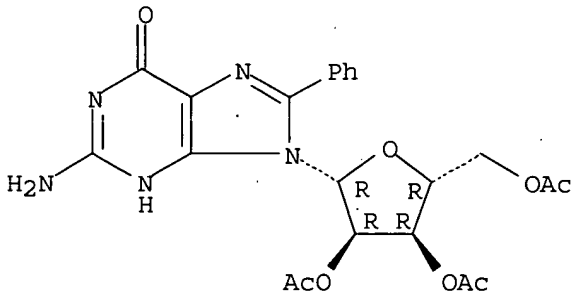
RN 172945-47-0 CAPLUS
CN Adenosine, 2'-deoxy-8-phenyl-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

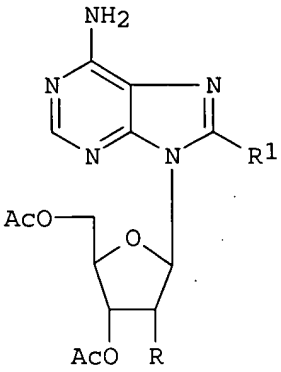


RN 172945-50-5 CAPLUS
CN Guanosine, 8-phenyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI

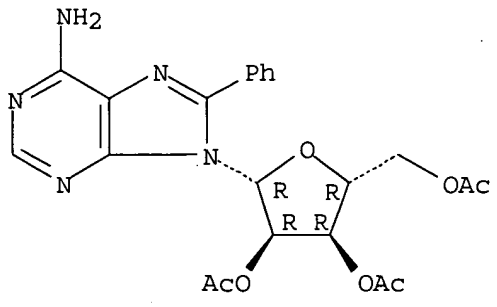


I

AB Palladium-catalyzed C-alkenylation of nucleosides, e.g. I (R = H, OAc, R1 = Br), with organotin R1SnR23 [R1 = Ph, CH2:CH, CH2:C(OEt), R2 = Me, Bu] gave the corresponding I [R = H, OAc, R1 = Ph, CH2:CH, CH2:C(OEt)] in good yields.

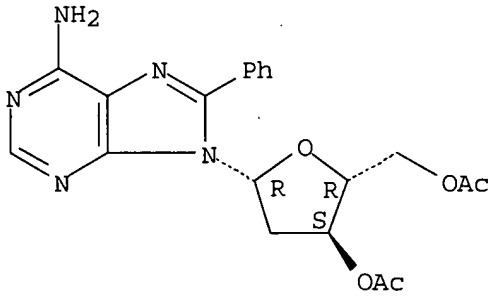
L4 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1995:897904 CAPLUS
DN 124:117836
TI Palladium catalysis in the synthesis of 8-position modified adenosine, 2'-deoxyadenosine and guanosine
AU Tu, Chi; Keane, Charlene; Eaton, Bruce E.
CS Medicinal Chemistry Department, Nexagen, Inc., Boulder, CO, 80301, USA
SO Nucleosides & Nucleotides (1995), 14(8), 1631-8
CODEN: NUNUD5; ISSN: 0732-8311
PB Dekker
DT Journal
LA English
OS CASREACT 124:117836
IT **172945-44-7P 172945-47-0P 172945-50-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium catalysis in synthesis of 8-position modified vinyl and aryl nucleosides)
RN 172945-44-7 CAPLUS
CN Adenosine, 8-phenyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



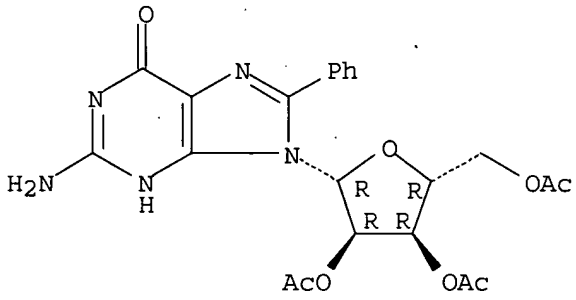
RN 172945-47-0 CAPLUS
CN Adenosine, 2'-deoxy-8-phenyl-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 172945-50-5 CAPLUS
CN Guanosine, 8-phenyl-, 2',3',5'-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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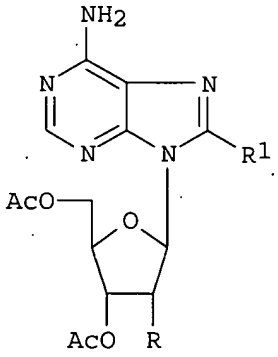


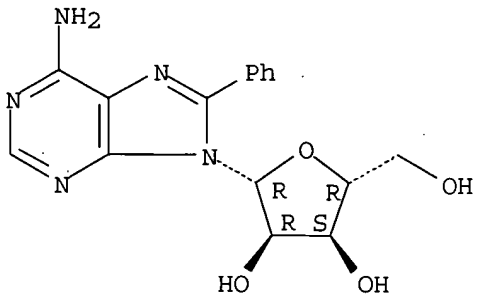
I

AB Adenosine and guanosine analogs with 8-position vinyl and aryl groups, e.g. I [R = H, OAc, R1 = Ph, CH:CH2, C(OEt):CH2], were prepd. by palladium catalyzed cross-coupling of organostannanes with 8-bromopurine nucleosides. The reaction conditions and catalyst compn. were improved so

that both vinyl and aryl modifications could be made by a general procedure.

L4 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1995:739235 CAPLUS
DN 123:187709
TI 8-Substituted adenosine and theophylline-7-riboside analogs as potential partial agonists for the adenosine A1 receptor
AU Van der Wenden, Eleonora M.; Hartog-Witte, Helen R.; Roelen, Harlof C. P. F.; von Frijtag Drabbe Kuenzel, Jacobien K.; Pirovano, Irene M.; Mathot, Ron A. A.; Danhof, Meindert; Van Aerschot, Arthur; Lidaks, Margeris J.; et al.
CS Division of Medicinal Chemistry, Leiden-Amsterdam Center for Drug Research, Leiden University, P.O. Box 9502, RA Leiden, 2300, Neth.
SO European Journal of Pharmacology, Molecular Pharmacology Section (1995), 290(3), 189-99
CODEN: EJPPET; ISSN: 0922-4106
PB Elsevier
DT Journal
LA English
IT **73340-78-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(structure activity of 8-substituted adenosine- and theophylline ribosides as A1 and A2A agonists)
RN 73340-78-0 CAPLUS
CN Adenosine, 8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

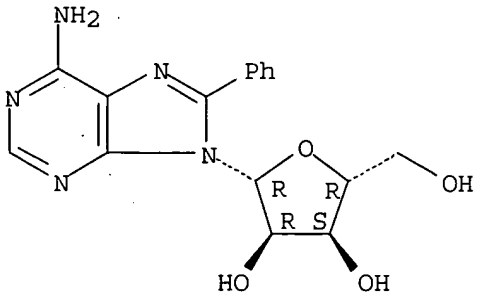


AB A series of 8-substituted adenosine and theophylline-7-riboside analogs (28 and 9 compds., resp.) was tested on adenosine A1 and A2A receptors as an extensive exploration of the adenosine C8-region. Alkylamino substituents at the 8-position cause an affinity decrease for adenosine analogs, but an affinity increase for theophylline-7-riboside derivs. The affinity decrease is probably due to a direct steric hindrance between the C8-substituent and the binding site as well as to electronic effects, not to a steric influence on the ribose moiety to adopt the anti conformation. The 8-substituents increase the affinity of theophylline-7-riboside analogs probably by binding to a lipophilic binding site. The intrinsic activity was tested in vitro for some 8-substituted adenosine analogs, by detg. the GTP shift in receptor binding studies and the inhibition of adenylate cyclase in a culture of rat thyroid FRTL-5 cells, and in vivo in the rat cardiovascular system for 8-butylaminoadenosine. Thus, it was shown that 8-ethyl-, 8-butyl-, and 8-pentylamino substituted analogs of adenosine may be partial agonists in vitro, and that 8-butylaminoadenosine

is a partial agonist for the rat cardiovascular A1 receptor in vivo.

L4 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1994:645130 CAPLUS
DN 121:245130
TI Selective Inhibition of Trypanosomal Glyceraldehyde-3-phosphate Dehydrogenase by Protein Structure-Based Design: Toward New Drugs for the Treatment of Sleeping Sickness
AU Verlinde, Christophe L. M. J.; Callens, Mia; Van Calenbergh, Serge; Van Aerschot, Arthur; Herdewijn, Piet; Hannaert, Veronique; Michels, Paul A. M.; Opperdoes, Fred R.; Hol, Wim G. J.
CS School of Medicine, University of Washington, Seattle, WA, 98195, USA
SO Journal of Medicinal Chemistry (1994), 37(21), 3605-13
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
IT **73340-78-0P**, 8-Phenyladenosine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein structure-based design of selective inhibition of glyceraldehyde phosphate dehydrogenase complexes of humans and Trypanosoma brucei in treatment of sleeping sickness)
RN 73340-78-0 CAPLUS
CN Adenosine, 8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

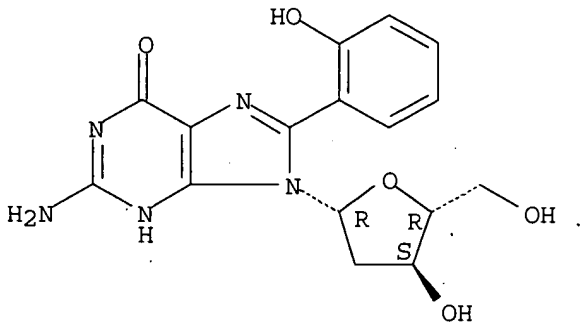


AB Within the framework of a project aimed at rational design of drugs against diseases caused by trypanosomes and related hemoflagellate parasites, selective inhibitors of trypanosomal glycolysis were designed, synthesized, and tested. The design was based upon the crystallog. detd. structures of the NAD:glyceraldehyde-3-phosphate dehydrogenase complexes of humans and Trypanosoma brucei, the causative agent of sleeping sickness. After one design cycle, using the adenosine part of the NAD cofactor as a lead, the following encouraging results were obtained: (1) a 2-Me substitution, targeted at a small pocket near Val 36, improves inhibition of the parasite enzyme 12.5-fold; (2) an 8-(thien-2-yl) substitution, aimed at Leu 112 of the parasite enzyme, where the equiv. residue in the mammalian enzyme is Val 100, results in a 167-fold better inhibition of the trypanosomal enzyme, while the inhibition of the human enzyme is improved only 13-fold; (3) exploitation of a "selectivity cleft" created by a unique backbone conformation in the trypanosomal enzyme near the adenosine ribose yields a considerable improvement in selectivity: 2'-deoxy-2'-(3-methoxybenzamido)adenosine e inhibits the human enzyme only

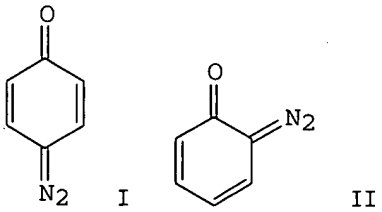
marginally but enhances inhibition of the parasite enzyme 45-fold when compared with adenosine. The designed inhibitors are not only better inhibitors of T. brucei GAPDH but also of the enzyme from Leishmania mexicana.

L4 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1992:506100 CAPLUS
DN 117:106100
TI Substitution of p- and o-hydroxyphenyl radicals at the 8-position of purine nucleosides by reaction with mutagenic p- and o-diazoquinones
AU Kikugawa, Kiyomi; Kato, Tetsuta; Kojima, Kazuhiro
CS Tokyo Coll. Pharm., Hachioji, 192-03, Japan
SO Mutation Research (1992), 268(1), 65-75
CODEN: MUREAV; ISSN: 0027-5107
DT Journal
LA English
IT **143084-41-7**
RL: BIOL (Biological study)
(as diazoquinone reaction product, mutagenicity in relation to)
RN 143084-41-7 CAPLUS
CN Guanosine, 2'-deoxy-8-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



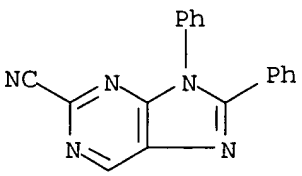
GI



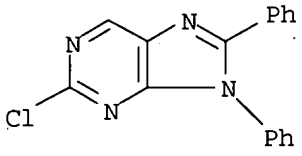
AB Incubation of 2'-deoxyadenosine (dAdo), 2'-deoxyguanosine (dGuo), adenosine, guanosine (Guo), thymidine, and deoxycytidine with p- and o-diazoquinones [pD (I) and oD (II), resp.], mutagens produced by the reaction of phenol and nitrate, at pH 7 and 37.degree. resulted in a decrease in each nucleoside depending upon the concn. of the diazoquinones. The pD-dAdo, pD-dGuo, and pD-Guo were isolated from the reaction mixts. of dAdo, dGuo, and Guo, resp., with p-diazoquinone at pH 9.5, and oD-dGuo was isolated from the mixt. of dGuo and o-diazoquinone at

pH 9.5. The products were identified as 8-(p-hydroxyphenyl)- and 8-(o-hydroxyphenyl)-purine nucleosides by 1H- and 13C-NMR spectra, secondary ion mass spectrum, UV absorption spectrum, and elemental anal. p- And o-diazoquinones may be converted into p- and o-hydroxyphenyl radicals, resp., which in turn attack the 8 position of the purine nucleosides. The mutagenicity of these diazoquinones may be partly due to the radical reactions.

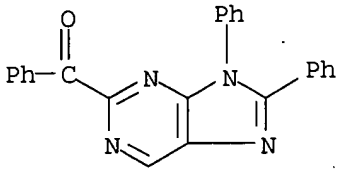
L4 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1990:514920 CAPLUS
DN 113:114920
TI Purines. IX. Reaction of 9-phenyl-9H-purine-2-carbonitriles with Grignard reagents
AU Tanji, Kenichi; Higashino, Takeo
CS Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
SO Heterocycles (1990), 30(1, Spec. Issue), 435-40
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
OS CASREACT 113:114920
IT **129006-37-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with Grignard reagents)
RN 129006-37-7 CAPLUS
CN 9H-Purine-2-carbonitrile, 8,9-diphenyl- (9CI) (CA INDEX NAME)



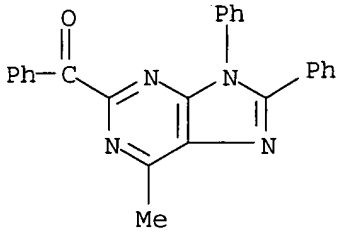
IT **129006-33-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with cyanide)
RN 129006-33-3 CAPLUS
CN 9H-Purine, 2-chloro-8,9-diphenyl- (9CI) (CA INDEX NAME)



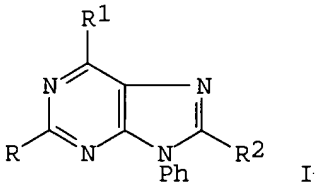
IT **129006-43-5P 129006-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 129006-43-5 CAPLUS
CN Methanone, (8,9-diphenyl-9H-purin-2-yl)phenyl- (9CI) (CA INDEX NAME)



RN 129006-44-6 CAPLUS
CN Methanone, (6-methyl-8,9-diphenyl-9H-purin-2-yl)phenyl- (9CI) (CA INDEX NAME)



GI

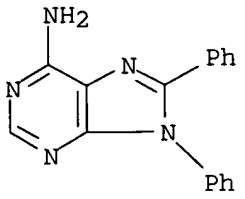


I

AB The Pd-catalyzed cross-coupling reaction of chlorophenylpurines I (R = Cl, R1 = H, Me, R2 = H, Ph; R = H, Me, R1 = Cl, R2 = H, Ph) with KCN proceeded to give purinecarbonitriles I (R = cyano, R1 = H, Me, R2 = H, Ph; R = H, Me, R1 = cyano, R2 = H, Ph). The conversion of I (R = cyano) into I (R = Ac, COEt, Bz) was achieved by treatment with Grignard reagents.

L4 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1990:458784 CAPLUS
DN 113:58784
TI Purine derivatives as competitive inhibitors of human erythrocyte membrane phosphatidylinositol 4-kinase
AU Young, Rodney C.; Jones, Martin; Milliner, Kevin J.; Rana, Kishore K.; Ward, John G.
CS Smith Kline and French Res. Ltd., Welwyn/Hertfordshire, AL6 9AR, UK
SO Journal of Medicinal Chemistry (1990), 33(8), 2073-80
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 113:58784
IT **127820-25-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphatidylinositol 4-kinase inhibition by)

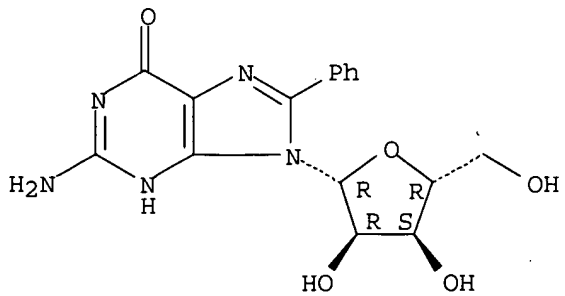
RN 127820-25-1 CAPLUS
CN 9H-Purin-6-amine, 8,9-diphenyl- (9CI) (CA INDEX NAME)



AB The possibility of deriving a potent, cell-penetrating inhibitor of human erythrocyte phosphatidylinositol 4-kinase, competitive with respect to ATP, has been investigated in a series of purine derivs. and analogs. The purine nucleus is not essential for binding to the ATP site but offers the advantage of synthetic accessibility to its derivs. The optimum substitution pattern in purine consisted of an electron-releasing substituent in the 6-position (e.g. amino, as in adenine) and a compact, lipophilic group in either the 8-position or, preferably, the 9-position, suggesting the importance of the N-1 lone pair and hydrophobic contributions of the 8- and 9-substituents to binding. The most potent inhibitor synthesized was 9-cyclohexyladenine, which has an apparent Ki value of 3.7 .mu.M.

L4 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1982:52623 CAPLUS
DN 96:52623
TI Reactions of benzenediazonium ions with guanine and its derivatives
AU Hung, Ming Hong; Stock, Leon M.
CS Dep. Chem., Univ. Chicago, Chicago, IL, 60637, USA
SO Journal of Organic Chemistry (1982), 47(3), 448-53
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
IT **79953-03-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
RN 79953-03-0 CAPLUS
CN Guanosine, 8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

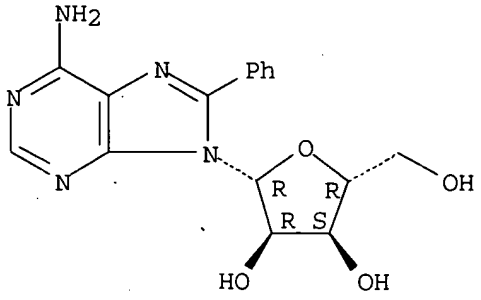


AB Guanine reacts with several benzenediazonium ions rapidly in aq. soln. at

pH 10.5 to form 8-(arylazo)guanines in good yield. The reaction of guanine with 4-bromobenzenediazonium ion forms 8-[(4-bromophenyl)azo]guanine about 50-fold more rapidly than the reaction of adenine with this ion to yield 6-[3-(4-bromophenyl)-2-triazen-1-yl]purine under these exptl. conditions. Guanosine reacts much more slowly than guanine with the benzenediazonium ions in aq. soln. at pH 8.5 or 10.5 to give 8-arylguanosines. The structures of these products were established by their spectroscopic properties and by their quant. conversion to 8-arylguanines. 5'-Guanylic acid also reacts quite slowly with the benzenediazonium ions in aq. soln. at pH 10.5. Only the compds. with strong electron-withdrawing groups yield N-2 triazenes at ambient temp. No 8-aryl or 8-arylazo compds. are formed with 5'-guanylic acid at this temp. However, 4-bromo- and 4-sulfobenzenediazonium ions react with 5'-guanylic acid at higher temps. to yield the 8-aryl-5'-guanylic acids in low yield. The structures of these products were proven by hydrolysis to 8-arylguanines. The 8-arylguanosines and the 8-aryl-5'-guanylic acids are formed via free-radical phenylation reactions. The factors governing the reactivity of the adenines and the guanines are discussed.

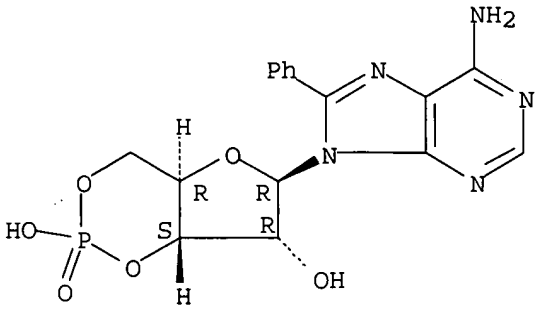
L4 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1980:164214 CAPLUS
DN 92:164214
TI Modification of position 8 of purine nucleosides and of adenosine 3',5'-cyclic monophosphate. Catalytic coupling reactions of organomagnesiums with 8-bromopurine riboside and 8-bromoadenosine 3',5'-cyclic monophosphate silyl derivatives in the presence of dichlorobis(triphenylphosphine)palladium
AU Nguyen Cong-Danh; Beaucourt, Jean Pierre; Pichat, Louis
CS Servi. Mol. Marquees, CEN-Saclay, Gif-sur-Yvette, F91190, Fr.
SO Tetrahedron Letters (1979), (34), 3159-62
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA French
IT **73340-78-0P 73340-84-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and silylation of)
RN 73340-78-0 CAPLUS
CN Adenosine, 8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



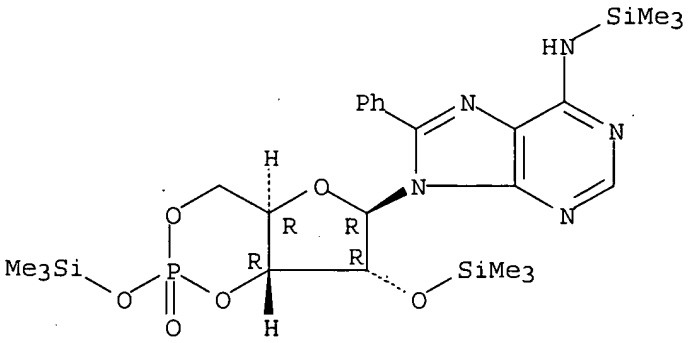
RN 73340-84-8 CAPLUS
CN Adenosine, 8-phenyl-, cyclic 3',5'-(hydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



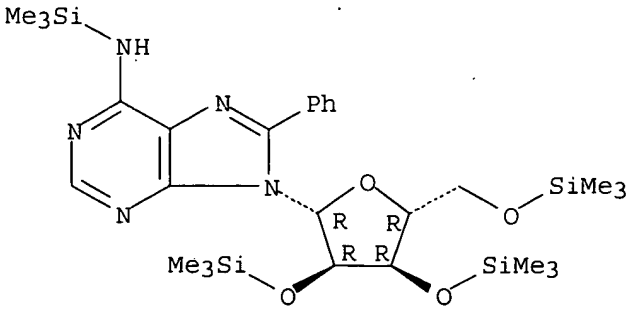
IT **73340-93-9P 73340-94-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 73340-93-9 CAPLUS
CN Adenosine, 8-phenyl-N-(trimethylsilyl)-2'-O-(trimethylsilyl)-, cyclic 3',5'-(trimethylsilyl phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

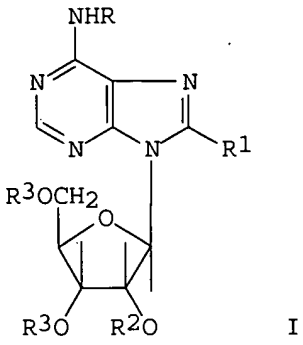


RN 73340-94-0 CAPLUS
CN Adenosine, 8-phenyl-N-(trimethylsilyl)-2',3',5'-tris-O-(trimethylsilyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI

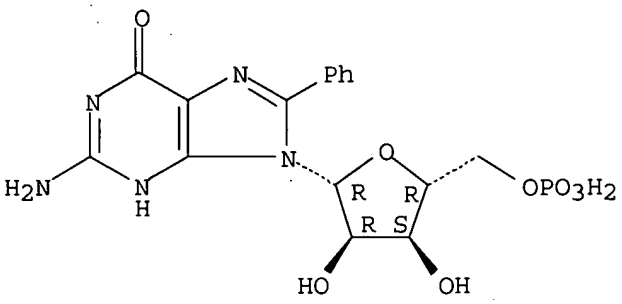


I

AB Pd catalyzed condensation of Grignard reagents with silyl derivs. of 8-bromoadenosine 3'5'-cyclic monophosphate is a convenient method for the prepn. of the corresponding 8-alkyl derivs. E.g., condensation of the purine I (R = R2 = R3 = SiMe3, R1 = Br) with CH2:CHCH2MgCl in THF, in the presence of (Ph3P)2PdCl2 gave, after hydrolysis, 35% I (R = R2 = R3 = H, R1 = CH2CH:CH2). Similar treatment of the cyclic phosphate I [R = R2 = SiMe3, R1 = Br, R32 = P(O)SiMe3] gave 30% I [R = R2 = H, R1 = CH2CH:CH2, R32 = P(O)OH]. In the latter reaction, changing the catalyst to Pd(PPh3)4 or (Ph3P)2NiCl2 had little effect on product yield.

L4 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2003 ACS
AN 1972:22084 CAPLUS
DN 76:22084
TI Reactions of carcinogens with guanine nucleotides
AU Hoffmann, Hans Dieter; Mueller, W.
CS Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed. Rep. Ger.
SO Phys.-Chem. Mech. Carcinog., Proc. Int. Symp. (1969), Meeting Date 1968, 183-7. Editor(s): Bergmann, E. D. Publisher: Isr. Acad. Sci. Hum., Jerusalem, Israel.
CODEN: 23XJAP
DT Conference
LA English
IT **35058-93-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35058-93-6 CAPLUS
CN 5'-Guanylic acid, 8-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Direct arylation of C-8 of guanine nucleotides was achieved by reaction with hydrocarbon radicals. X-irradn. of a DNA soln. satd. with benzo[a]pyrene yielded 8-benzo[a]pyrenylguanine. 5'-GMP and phenyldimethyltriazene gave 8-phenylguanosine 5'-phosphate. Reaction of DNA with the hydroxylamino free radical of nitroquinoline N-oxide followed by hydrolysis by DNase gave the same product as the direct reaction of the guanine nucleotide, but the quinoline-substituted guanine was not synthesized. Such modifications of DNA may hinder the binding of repressor mols.

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L6             0 L5
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